Mean pKa Result

Multiset name: **0417936-0002**   Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_ISA_H2O_05_22_18.t3r**

Mean pKa result

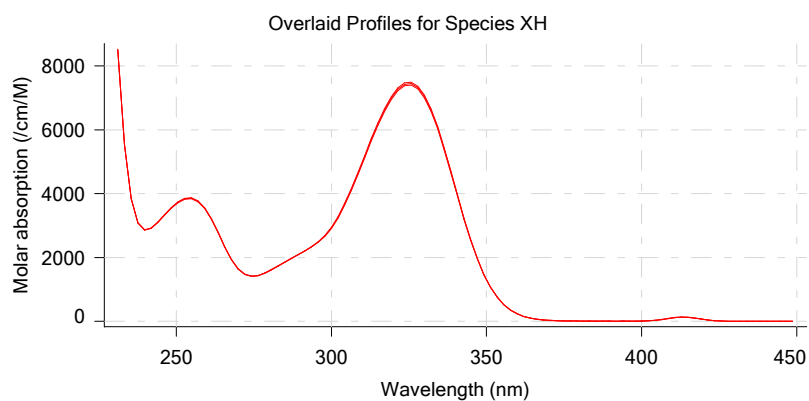| pKa	Std Dev	Ionic strength	Temperature
4.83	0.018	0.155 M	24.9°C
8.86	0.013	0.155 M	24.9°C

Warnings and errors

Errors   None
Warnings   None

Mean pKa individual results

Titration	Direction	Ionic strength	Temperature	Chi Squared	pKa 1		pKa 2
18E-22003 Points 4 to 27	Up	0.156 M	24.9°C	0.0493	☑	4.81 ☑	8.85
18E-22004 Points 4 to 36	Up	0.155 M	24.9°C	0.0453	☑	4.83 ☑	8.87
18E-22010 Points 4 to 38	Up	0.155 M	24.9°C	0.0383	☑	4.84 ☑	8.86

Graphs
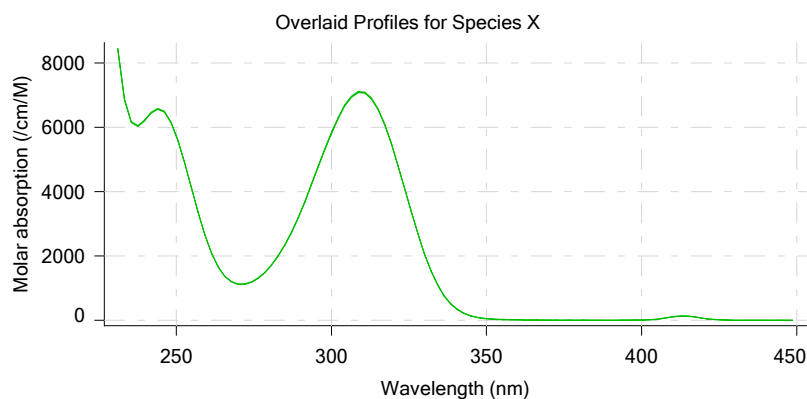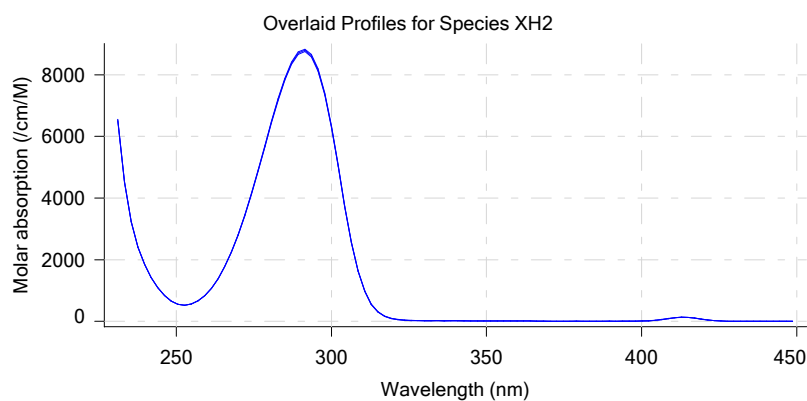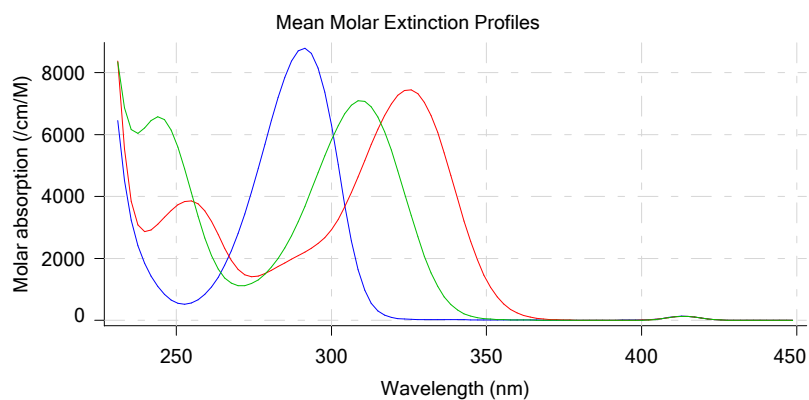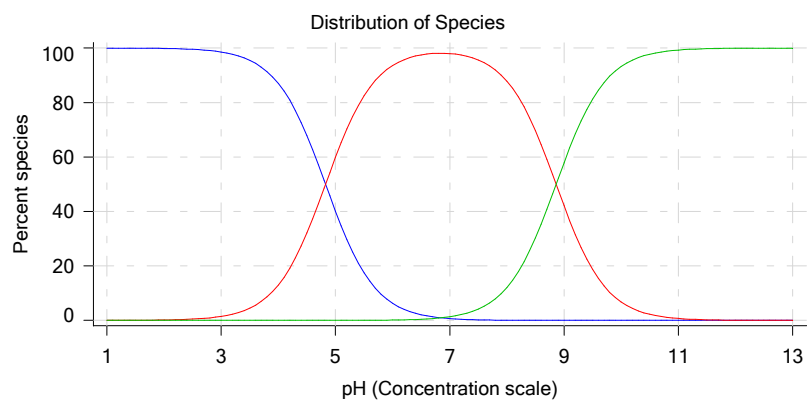
Distribution of Species

Mean Molar Extinction Profiles

Overlaid Profiles for Species XH2

Overlaid Profiles for Species XH

Overlaid Profiles for Species X

Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_ISA_H2O_05_22_18.t3r**

Multiset assays

Assay 1 of 3
Sample name	UV-metric pKa_0417936-0002
Assay name	UV-metric pKa
Assay ID	18E-22003
Instrument ID	T311053
Imported from	C:\Sirius_T3\18E-22003_Pyridoxine HCl_UV-metric pKa_0417936-0002.t3r
Imported on	5/22/2018 1:54:49 PM
Analyst name	Dorothy Levorse
Experiment start time	5/22/2018 9:47:33 AM

Assay 2 of 3
Sample name	UV-metric pKa_0417936-0002
Assay name	UV-metric pKa
Assay ID	18E-22004
Instrument ID	T311053
Imported from	C:\Sirius_T3\18E-22004_Pyridoxine HCl_UV-metric pKa_0417936-0002.t3r
Imported on	5/22/2018 1:54:49 PM
Analyst name	Dorothy Levorse
Experiment start time	5/22/2018 10:11:10 AM

Assay 3 of 3
Sample name	UV-metric pKa_0417936-0002
Assay name	UV-metric pKa
Assay ID	18E-22010
Instrument ID	T311053
Imported from	C:\Sirius_T3\18E-22010_Pyridoxine HCl_UV-metric pKa_0417936-0002.t3r
Imported on	5/22/2018 1:54:49 PM
Analyst name	Dorothy Levorse
Experiment start time	5/22/2018 11:56:49 AM

UV-metric pKa_0417936-0002   Titration 1 of 1   18E-22003 Points 4 to 27

Results

pKa 1	**4.81**
pKa 2	**8.85**
RMSD	**0.005 0.004 0.007**
Chi squared	**0.0493**
PCA calculated number of pKas	**1**
Average ionic strength	**0.156 M**
Average temperature	**24.9°C**
Analyte concentration range	**61.7 µM to 57.7 µM**
Number of pKas source	**Predicted**
Wavelength clipping	**230.0 nm to 450.0 nm**
pH clipping	**1.459 to 12.518**

Warnings and errors

Errors   None
Warnings   PCA calculation disagrees with predicted number of pKas

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
Buffer in use	Yes			
Buffer type	Phosphate Buffer			
Assay Medium				
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			

UV-metric pKa

Multiset name: **0417936-0002**   Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_ISA_H2O_05_22_18.t3r**

Graphs

Spectral Data by Wavelength

Spectral Data by Wavelength

Spectral Data by Wavelength

Spectral Data by Wavelength

Spectral Data by Wavelength

Spectral Data by pH

Spectral Data by pH

Spectral Data by pH

UV-metric pKa

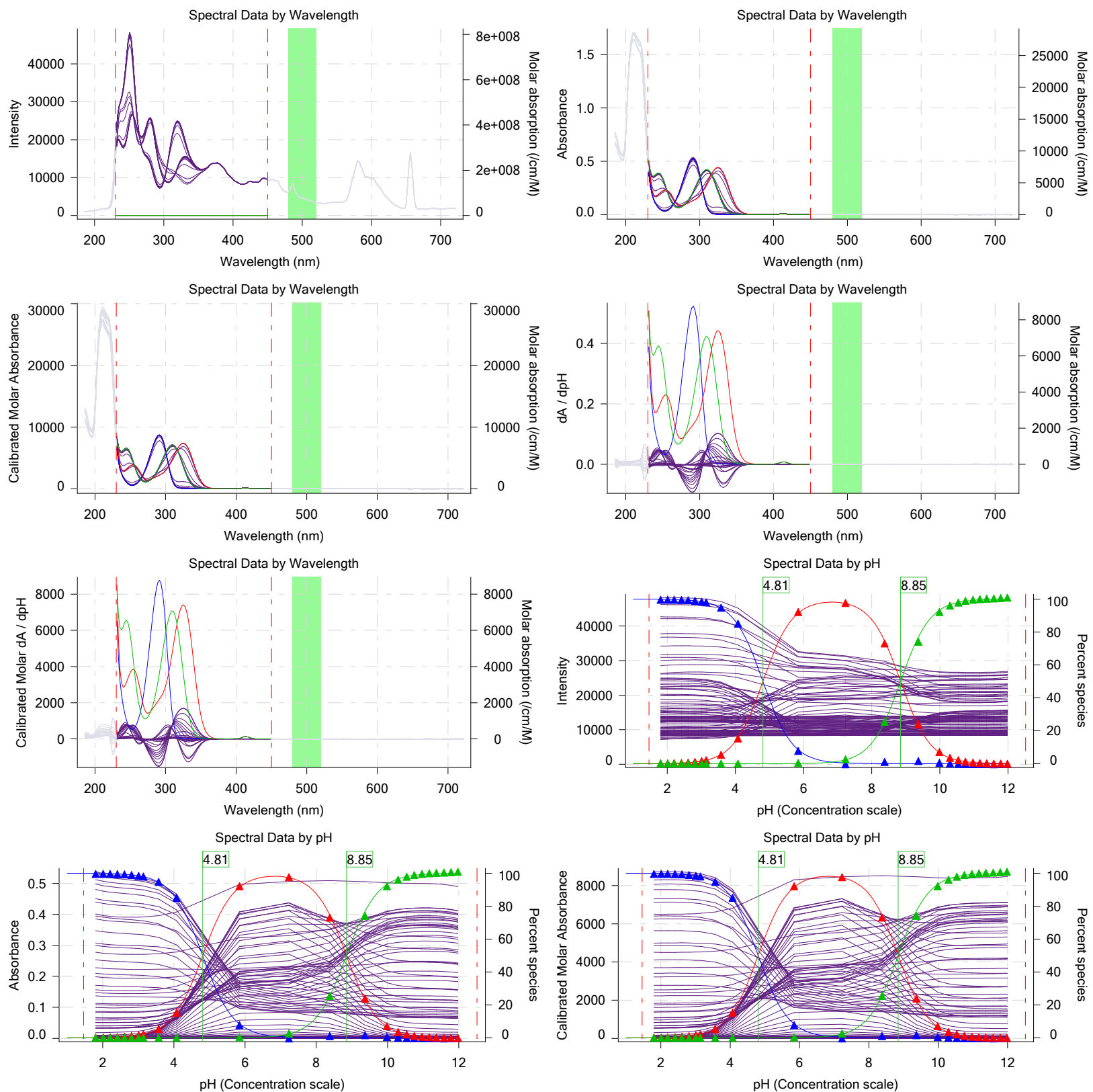Multiset name: **0417936-0002**   Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
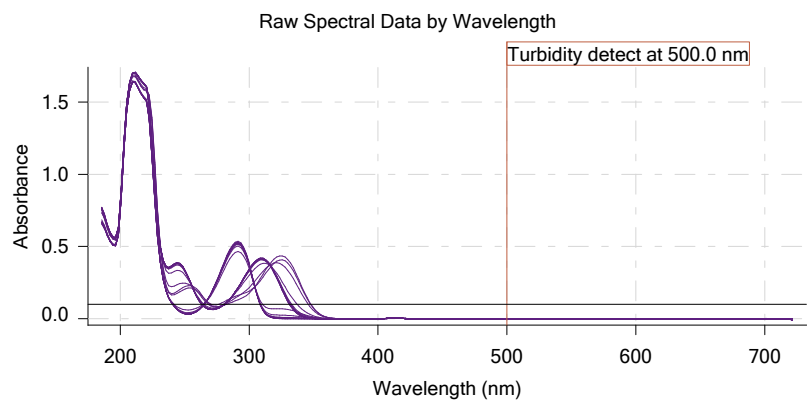Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_ISA_H2O_05_22_18.t3r**

Graphs (continued)

Spectral Data by pH

Spectral Data by pH

PCA Results

Distribution of Species

Molar Absorption Profile

Baseline Correction Range

Raw Spectral Data by Wavelength

Turbidity detect at 500.0 nm

UV-metric pKa_0417936-0002   18E-22003   Assay 1 of 3

Multiset name: **0417936-0002**   Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
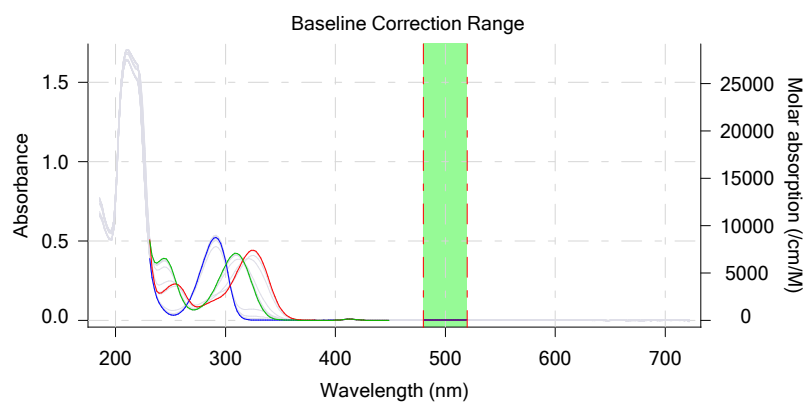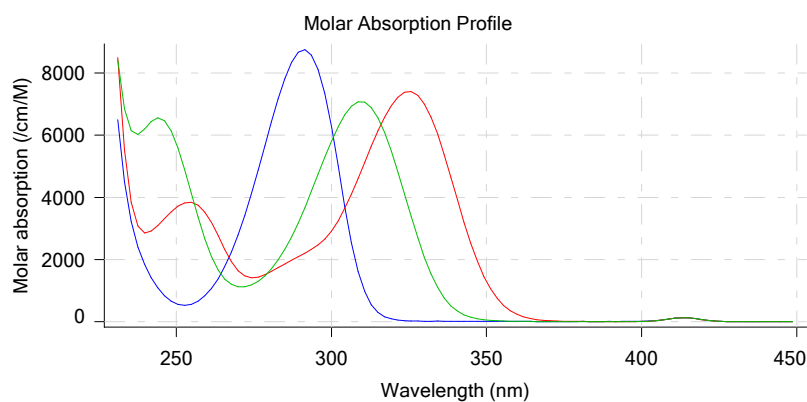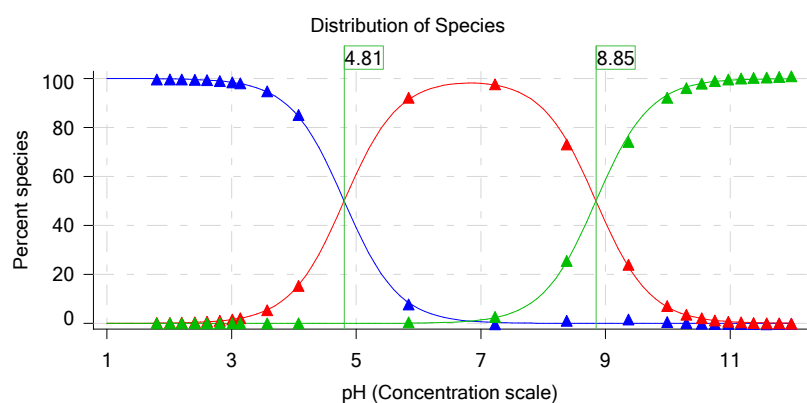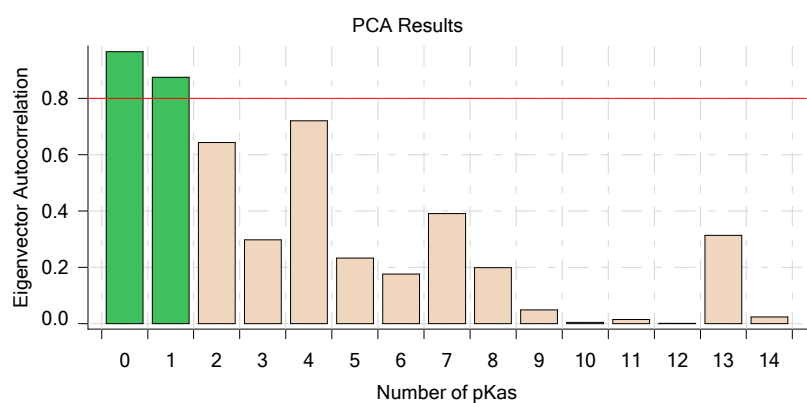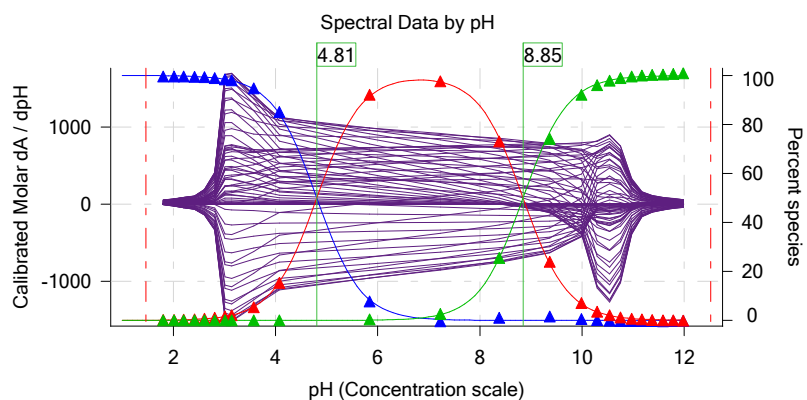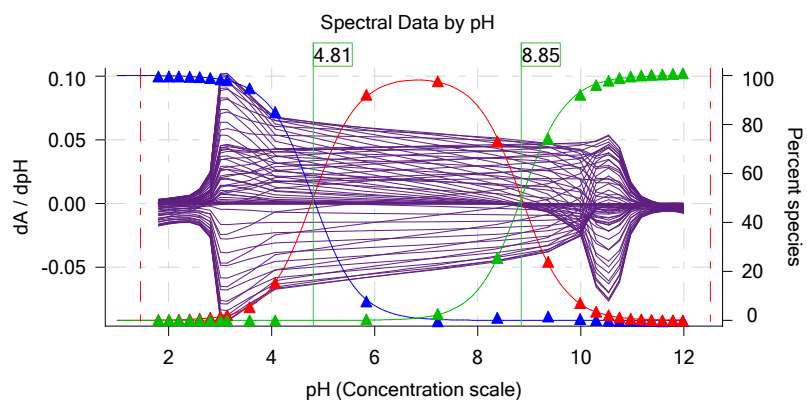Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_ISA_H2O_05_22_18.t3r**

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	Pyridoxine HCl	5/22/2018 9:07:27 AM	User entered value
Sample by	Volume		Default value
Sample volume	0.0020 mL	5/22/2018 9:07:27 AM	User entered value
Solvent	DMSO		Default value
Sample concentration	0.048630 M	5/22/2018 9:07:27 AM	User entered value
Solubility	Unknown		Default value
Molecular weight	205.64	5/22/2018 9:07:35 AM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	2	5/22/2018 9:07:27 AM	User entered value
Sample is a	Ampholyte	5/22/2018 9:07:27 AM	User entered value
pKa 1	4.90	5/22/2018 9:07:27 AM	User entered value
Type	Base	5/22/2018 9:07:27 AM	User entered value
pKa 2	8.80	5/22/2018 9:07:27 AM	User entered value
Type	Acid	5/22/2018 9:07:27 AM	User entered value
logp (XH2 +)	-10.00		Default value
logP (neutral XH)	-10.00	5/22/2018 9:07:27 AM	User entered value
logP (X -)	-10.00		Default value
Stoichiometry	1.00000		Default value
Aprotic counterion name	Chloride		From standards.xml file
Stoichiometry	1.00		From standards.xml file
Charge per counterion	-1		From standards.xml file

Events

Time	Event	Water	Acid	Base	Buffer	pH	dpH/dt	pH R-squared	pH SD
3:33.0	Dark spectrum								
3:34.5	Reference spectrum								
4:02.1	Volume reset due to vial change								
5:32.5	Initial pH = 7.00								
6:42.6	Data point 4	1.50000 mL	0.05005 mL	0.00000 mL	0.02500 mL	1.959	-0.00887	0.73649	0.000
7:11.4	Data point 5	1.50000 mL	0.05005 mL	0.01889 mL	0.02500 mL	2.160	0.01734	0.75340	0.000
7:28.3	Data point 6	1.50000 mL	0.05005 mL	0.03041 mL	0.02500 mL	2.346	0.02477	0.93085	0.001
7:45.2	Data point 7	1.50000 mL	0.05005 mL	0.03789 mL	0.02500 mL	2.552	0.02775	0.97111	0.001
8:02.0	Data point 8	1.50000 mL	0.05005 mL	0.04245 mL	0.02500 mL	2.743	0.02913	0.95284	0.001
8:18.7	Data point 9	1.50000 mL	0.05005 mL	0.04537 mL	0.02500 mL	2.945	0.03866	0.89439	0.002
8:35.4	Data point 10	1.50000 mL	0.05005 mL	0.04718 mL	0.02500 mL	3.140	0.09720	0.93849	0.004
8:52.1	Data point 11	1.50000 mL	0.05005 mL	0.04831 mL	0.02500 mL	3.269	0.08258	0.96765	0.004
9:13.8	Data point 12	1.50000 mL	0.05005 mL	0.04988 mL	0.02500 mL	3.698	0.10062	0.98900	0.004
9:53.2	Data point 13	1.50000 mL	0.05005 mL	0.05049 mL	0.02500 mL	4.193	0.13230	0.98440	0.006
11:10.0	Data point 14	1.50000 mL	0.05005 mL	0.05108 mL	0.02500 mL	5.946	0.33161	0.98757	0.016
12:31.9	Data point 15	1.50000 mL	0.05005 mL	0.05158 mL	0.02500 mL	7.318	0.20496	0.99721	0.010
14:04.3	Data point 16	1.50000 mL	0.05005 mL	0.05191 mL	0.02500 mL	8.458	0.32628	0.99345	0.016
15:26.3	Data point 17	1.50000 mL	0.05005 mL	0.05221 mL	0.02500 mL	9.440	0.09863	0.99096	0.004
16:35.1	Data point 18	1.50000 mL	0.05005 mL	0.05270 mL	0.02500 mL	10.052	0.09577	0.95968	0.004
17:16.4	Data point 19	1.50000 mL	0.05005 mL	0.05334 mL	0.02500 mL	10.358	0.09826	0.98862	0.004
17:53.7	Data point 20	1.50000 mL	0.05005 mL	0.05430 mL	0.02500 mL	10.599	0.09994	0.98671	0.004
18:28.9	Data point 21	1.50000 mL	0.05005 mL	0.05564 mL	0.02500 mL	10.809	0.04418	0.96809	0.002
19:01.1	Data point 22	1.50000 mL	0.05005 mL	0.05802 mL	0.02500 mL	11.025	0.03427	0.91032	0.001
19:28.1	Data point 23	1.50000 mL	0.05005 mL	0.06098 mL	0.02500 mL	11.227	0.02827	0.97094	0.001
19:44.9	Data point 24	1.50000 mL	0.05005 mL	0.06585 mL	0.02500 mL	11.422	0.01501	0.81297	0.000
20:01.7	Data point 25	1.50000 mL	0.05005 mL	0.07364 mL	0.02500 mL	11.631	0.00685	0.73754	0.000
20:18.7	Data point 26	1.50000 mL	0.05005 mL	0.08648 mL	0.02500 mL	11.829	0.01037	0.87129	0.000
20:35.9	Data point 27	1.50000 mL	0.05005 mL	0.10727 mL	0.02500 mL	12.018	0.01161	0.73671	0.000
22:34.8	Assay volumes	1.75000 mL	0.16103 mL	0.10727 mL	0.02500 mL				

Multiset name: **0417936-0002**   Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_ISA_H2O_05_22_18.t3r**

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				
Analyst name	Dorothy Levorse			
Separate reference vial	Yes			
Standard Experiment Settings				
Number of titrations	1			
Minimum pH	2.000			
Maximum pH	12.000			
pH step between points of	0.200			
Minimum titrant addition	0.00002 mL			
Maximum titrant addition	0.10000 mL			
Argon flow rate	100%			
Start titration using	Cautious pH adjust			
Advanced General Settings				
Detect turbidity using	Spectrometer			
Monitor at a wavelength of	500.0 nm			
Absorbance threshold of	0.100			
Collect turbidity sensor data	No			
Stir after titrant addition for	5 seconds			
For titrant addition, stir at	15%			
Titrant Pre-Dose				
Titrant pre-dose	None			
Assay Medium				
Cosolvent in use	No			
ISA water volume	1.50 mL			
Water added	Automatic			
After water addition, stir for	5 seconds			
At a speed of	15%			
Buffer in use	Yes			
Buffer type	Phosphate Buffer			
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			
After medium addition, stir for	5 seconds			
Sample Sonication				
Sonicate	No			
Sample Dissolution				
Perform a dissolution stage	No			
Carbonate purge				
Perform a carbonate purge	No			
Temperature Control				
Wait for temperature	Yes			
Required start temperature	25.0°C			
Acceptable deviation	0.5°C			
Time to wait	60 seconds			
Stir speed of	15%			
Titration 1				
Titrate from	Low to high pH			
Adjust to start pH	Yes			
After pH adjust stir for	10 seconds			
Data Point Stability				
Stir during data point collection	Yes			
For point collection, stir at	15%			
Delay before data point collection	0 seconds			
Number of points to average	20 points			
Time interval between points	0.50 seconds			
Required maximum standard deviation	0.00500 dpH/dt			
Stability timeout after	60 seconds			
Experiment cleanup				
Adjust pH to cleanup	To start pH			
And then stir for	60 seconds			

Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_ISA_H2O_05_22_18.t3r**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
For cleaning, stir at	20%			
Then add water volume	0.25 mL			
And then stir for	30 seconds			

Calibration Settings

Setting	Value	Date/Time changed	Imported from
Four-Plus alpha	0.160	5/22/2018 9:47:32 AM	C:\Sirius_T3\18E-21006_Blank standardisation.t3r
Four-Plus S	0.9904	5/22/2018 9:47:32 AM	C:\Sirius_T3\18E-21006_Blank standardisation.t3r
Four-Plus jH	1.0	5/22/2018 9:47:32 AM	C:\Sirius_T3\18E-21006_Blank standardisation.t3r
Four-Plus jOH	-0.5	5/22/2018 9:47:32 AM	C:\Sirius_T3\18E-21006_Blank standardisation.t3r
Base concentration factor	1.012	5/22/2018 9:47:33 AM	C:\Sirius_T3\KOH18D10.t3r
Acid concentration factor	1.011	5/22/2018 9:47:33 AM	C:\Sirius_T3\18E-21006_Blank standardisation.t3r

Instrument Settings

Setting	Value	Batch Id	Install date
Instrument owner	Merck		
Instrument ID	T311053		
Instrument type	T3 Simulator		
Software version	1.1.3.0		
Dispenser module		T3DM1100253	3/31/2009 6:24:52 AM
Dispenser 0	Water		3/31/2009 6:25:05 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Water (0.15 M KCl)	2-6-18	5/15/2018 2:12:22 PM
Dispenser 2	Acid		3/31/2009 6:25:11 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Acid (0.5 M HCl)	3-22-18	5/15/2018 2:12:48 PM
Dispenser 1	Base		3/31/2009 6:25:21 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Base (0.5 M KOH)	3-22-18	5/15/2018 2:12:34 PM
Dispenser 5	Cosolvent		3/31/2009 6:26:24 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Distribution valve 5	Distribution Valve		3/31/2009 6:28:19 AM
Firmware version	1.1.3		
Port A	Methanol (80%, 0.15 M KCl)	2-8-18	5/15/2018 2:14:14 PM
Port B	Cyclohexane		4/10/2018 8:40:51 AM
Port C	MeCN (50%, 0.15 M KCl)	4-16-18	5/15/2018 2:14:20 PM
Dispenser 3	Buffer		8/3/2010 6:05:16 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Dodecane	1-31-2018	5/15/2018 2:12:54 PM
Dispenser 6	Octanol		10/22/2010 11:52:43 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Octanol	1-31-2018	4/9/2018 9:14:11 AM
Titrator		T3TM1100153	3/31/2009 6:24:17 AM
Horizontal axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Probe I/O firmware version	1.1.1		
Electrode	T3 Electrode	T3E0769	8/15/2017 10:21:54 AM
E0 calibration	-9.65 mV		5/22/2018 9:48:00 AM
Filling solution	3M KCl	KCL095	5/21/2018 8:57:01 AM
Liquids			
Wash 1	50% IPA:50% Water		5/22/2018 8:38:15 AM

Multiset name: **0417936-0002**

Instrument ID: **T311053**

Analyst: **Dorothy Levorse**

Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_ISA_H2O_05_22_18.t3r**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Wash 2	0.5% Trition X-100 in H20		5/22/2018 8:38:18 AM
Buffer position 1	pH7 Wash		5/22/2018 8:38:22 AM
Buffer position 2	pH 7		5/22/2018 8:38:25 AM
Storage position			5/22/2018 8:38:32 AM
Wash water	3.9e+003 mL	5-15-18	5/15/2018 2:11:48 PM
Waste	6.6e+003 mL		3/19/2018 10:48:12 AM
Temperature controller			8/5/2010 7:35:13 AM
Turbidity detector			3/31/2009 6:24:45 AM
Spectrometer		072390	11/23/2010 12:22:28 PM
Dip probe		11086	
Wavelength coefficient A0	185.563		
Wavelength coefficient A1	2.17439		
Wavelength coefficient A2	-0.000285622		
Total lamp lit time	897:26:49		11/23/2010 12:22:28 PM
Calibrated on	5/21/2018 2:44:22 PM		
Integration time	19		
Scans averaged	10		
Autoloader		T3AL1100237	11/10/2015 10:34:13 AM
Left-right axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Front-back axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Configuration			
Alternate titration position	Titration position		
Alternate reference position	Reference position		
Maximum standard vial volume	3.50 mL		
Maximum alternate vial volume	25.00 mL		
Automatic action idle period	5 minute(s)		
Titrant tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		
Flowing wash stir speed	30%		
Solvent wash stir duration	5 s		
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		
E0 calibration reading stir speed	0%		
Spectrometer calibration stir duration	5 s		
Spectrometer calibration stir speed	30%		
Spectrometer calibration wash pump volume	20.0 mL		
Spectrometer calibration wash stir duration	5 s		
Spectrometer calibration wash stir speed	30%		
Overhead dispense height	10000		

Refinement Settings

Setting	Value	Default value
Turbidity detection method	Spectrometer	Spectrometer
Turbidity wavelength to assess	500.0 nm	500.0 nm
Turbidity maximum absorbance	0.100	0.100
Turbidity probe threshold	50.00	50.00

Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_ISA_H2O_05_22_18.t3r**

Refinement Settings (continued)

Setting	Value	Default value
Exclude turbid points	Yes	Yes
Low intensity warning threshold	100	100
Minimum absorbance change threshold	0.100	0.100
Eigenvector autocorrelation threshold	0.80	0.80
Maximum RMSD severe warning	0.250	0.250
Maximum RMSD warning	0.050	0.050

Experiment Log

[2:13] Air gap created for Water (0.15 M KCl)
[2:14] Air gap created for Acid (0.5 M HCl)
[2:14] Air gap created for Base (0.5 M KOH)
[2:15] Air gap created for Methanol (80%, 0.15 M KCl)
[2:15] Air gap released for Water (0.15 M KCl)
[2:19] Titrator arm moved to Reference position
[2:19] Argon flow rate set to 100
[2:19] Preparing reference vial
[2:19] Automatically add 1.50000 mL of water
[2:45] Dispensed 1.500000 mL of Water (0.15 M KCl)
[2:45] Stirrer speed set to 15
[2:55] Iterative adjust 7.73 -> 2.00
[2:55] pH 7.73 -> 2.00
[2:56] Air gap released for Acid (0.5 M HCl)
[2:57] Dispensed 0.043744 mL of Acid (0.5 M HCl)
[3:02] pH 2.06 -> 2.00
[3:02] Dispensed 0.006303 mL of Acid (0.5 M HCl)
[3:07] Stirrer speed set to 0
[3:11] Titrator arm moved over Reference position
[3:12] Air gap created for Water (0.15 M KCl)
[3:12] Air gap created for Acid (0.5 M HCl)
[3:16] Titrator arm moved to Reference position
[3:16] Air gap released for Water (0.15 M KCl)
[3:16] Stirrer speed set to 15
[3:31] Stirrer speed set to 0
[3:33] Dark scan collected
[3:34] Reference scan collected
[4:02] Probes washed
[4:02] Volume reset due to vial change
[4:10] Titrator arm moved to Titration position
[4:10] Preparing sample vial
[4:10] Automatically add 1.50000 mL of water
[5:22] Dispensed 1.500000 mL of Water (0.15 M KCl)
[5:22] Stirrer speed set to 15
[5:32] Initial pH = 7.00
[5:32] Adding reagent volumes used in reference
[5:32]   Adding acid volume of 0.0500470
[5:34] Air gap released for Acid (0.5 M HCl)
[5:35] Dispensed 0.050047 mL of Acid (0.5 M HCl)
[6:54] Datapoint id 4 collected
[6:54] pH 1.96 -> 2.16
[6:54] Using cautious pH adjust
[6:54] Air gap released for Base (0.5 M KOH)
[6:55] Dispensed 0.009360 mL of Base (0.5 M KOH)
[7:00] Stepping pH = 2.04
[7:01] Dispensed 0.007573 mL of Base (0.5 M KOH)
[7:06] Stepping pH = 2.13
[7:06] Dispensed 0.001952 mL of Base (0.5 M KOH)
[7:11] Stepping pH = 2.16
[7:22] Datapoint id 5 collected

Multiset name: **0417936-0002**　　　　　　　　　　　　　　Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_ISA_H2O_05_22_18.t3r**

Experiment Log (continued)

[7:22] Charge balance equation is out by 0.7%
[7:22] pH 2.16 -> 2.36
[7:22] Using charge balance adjust
[7:23] Dispensed 0.011524 mL of Base (0.5 M KOH)
[7:39] Datapoint id 6 collected
[7:39] Charge balance equation is out by -7.0%
[7:39] pH 2.35 -> 2.55
[7:39] Using charge balance adjust
[7:40] Dispensed 0.007479 mL of Base (0.5 M KOH)
[7:56] Datapoint id 7 collected
[7:56] Charge balance equation is out by 2.8%
[7:56] pH 2.55 -> 2.75
[7:56] Using charge balance adjust
[7:56] Dispensed 0.004563 mL of Base (0.5 M KOH)
[8:13] Datapoint id 8 collected
[8:13] Charge balance equation is out by -4.2%
[8:13] pH 2.74 -> 2.94
[8:13] Using charge balance adjust
[8:13] Dispensed 0.002916 mL of Base (0.5 M KOH)
[8:30] Datapoint id 9 collected
[8:30] Charge balance equation is out by 0.7%
[8:30] pH 2.94 -> 3.14
[8:30] Using charge balance adjust
[8:30] Dispensed 0.001811 mL of Base (0.5 M KOH)
[8:46] Datapoint id 10 collected
[8:46] Charge balance equation is out by -2.2%
[8:46] pH 3.14 -> 3.34
[8:46] Using charge balance adjust
[8:47] Dispensed 0.001129 mL of Base (0.5 M KOH)
[9:03] Datapoint id 11 collected
[9:03] Charge balance equation is out by -35.8%
[9:03] pH 3.27 -> 3.47
[9:03] Using cautious pH adjust
[9:03] Dispensed 0.000423 mL of Base (0.5 M KOH)
[9:08] Stepping pH = 3.29
[9:08] Dispensed 0.001152 mL of Base (0.5 M KOH)
[9:13] Stepping pH = 3.61
[9:42] Datapoint id 12 collected
[9:42] Charge balance equation is out by 80.2%
[9:42] pH 3.70 -> 3.90
[9:42] Using cautious pH adjust
[9:42] Dispensed 0.000165 mL of Base (0.5 M KOH)
[9:48] Stepping pH = 3.71
[9:48] Dispensed 0.000447 mL of Base (0.5 M KOH)
[9:53] Stepping pH = 3.97
[10:54] Datapoint id 13 collected
[10:54] Charge balance equation is out by 81.8%
[10:54] pH 4.19 -> 4.39
[10:54] Using cautious pH adjust
[10:54] Dispensed 0.000047 mL of Base (0.5 M KOH)
[10:59] Stepping pH = 4.22
[10:59] Dispensed 0.000141 mL of Base (0.5 M KOH)
[11:04] Stepping pH = 4.24
[11:05] Dispensed 0.000400 mL of Base (0.5 M KOH)
[11:10] Stepping pH = 5.13
[12:11] Datapoint id 14 collected
[12:11] Charge balance equation is out by 409.4%
[12:11] pH 5.95 -> 6.15
[12:11] Using cautious pH adjust
[12:11] Dispensed 0.000024 mL of Base (0.5 M KOH)

Multiset name: **0417936-0002**   Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_ISA_H2O_05_22_18.t3r**

Experiment Log (continued)

[12:16] Stepping pH = 6.00
[12:16] Dispensed 0.000047 mL of Base (0.5 M KOH)
[12:21] Stepping pH = 6.01
[12:21] Dispensed 0.000141 mL of Base (0.5 M KOH)
[12:26] Stepping pH = 6.03
[12:26] Dispensed 0.000282 mL of Base (0.5 M KOH)
[12:32] Stepping pH = 6.83
[13:33] Datapoint id 15 collected
[13:33] Charge balance equation is out by 1,013.5%
[13:33] pH 7.32 -> 7.52
[13:33] Using cautious pH adjust
[13:33] Dispensed 0.000024 mL of Base (0.5 M KOH)
[13:38] Stepping pH = 7.36
[13:38] Dispensed 0.000024 mL of Base (0.5 M KOH)
[13:43] Stepping pH = 7.38
[13:43] Dispensed 0.000024 mL of Base (0.5 M KOH)
[13:48] Stepping pH = 7.40
[13:49] Dispensed 0.000071 mL of Base (0.5 M KOH)
[13:54] Stepping pH = 7.42
[13:54] Dispensed 0.000165 mL of Base (0.5 M KOH)
[13:59] Stepping pH = 7.51
[13:59] Dispensed 0.000024 mL of Base (0.5 M KOH)
[14:04] Stepping pH = 7.62
[15:05] Datapoint id 16 collected
[15:05] Charge balance equation is out by 2,712.5%
[15:05] pH 8.46 -> 8.66
[15:05] Using cautious pH adjust
[15:05] Dispensed 0.000024 mL of Base (0.5 M KOH)
[15:11] Stepping pH = 8.51
[15:11] Dispensed 0.000024 mL of Base (0.5 M KOH)
[15:16] Stepping pH = 8.53
[15:16] Dispensed 0.000094 mL of Base (0.5 M KOH)
[15:21] Stepping pH = 8.56
[15:21] Dispensed 0.000165 mL of Base (0.5 M KOH)
[15:26] Stepping pH = 8.86
[16:19] Datapoint id 17 collected
[16:19] Charge balance equation is out by 815.6%
[16:19] pH 9.44 -> 9.64
[16:19] Using cautious pH adjust
[16:19] Dispensed 0.000047 mL of Base (0.5 M KOH)
[16:25] Stepping pH = 9.45
[16:25] Dispensed 0.000165 mL of Base (0.5 M KOH)
[16:30] Stepping pH = 9.50
[16:30] Dispensed 0.000282 mL of Base (0.5 M KOH)
[16:35] Stepping pH = 9.95
[17:06] Datapoint id 18 collected
[17:06] Charge balance equation is out by 329.6%
[17:06] pH 10.05 -> 10.25
[17:06] Using cautious pH adjust
[17:06] Dispensed 0.000165 mL of Base (0.5 M KOH)
[17:11] Stepping pH = 10.07
[17:11] Dispensed 0.000470 mL of Base (0.5 M KOH)
[17:16] Stepping pH = 10.31
[17:43] Datapoint id 19 collected
[17:43] Charge balance equation is out by 84.0%
[17:43] pH 10.36 -> 10.56
[17:43] Using cautious pH adjust
[17:43] Dispensed 0.000329 mL of Base (0.5 M KOH)
[17:48] Stepping pH = 10.40
[17:48] Dispensed 0.000635 mL of Base (0.5 M KOH)

Multiset name: **0417936-0002**   Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_ISA_H2O_05_22_18.t3r**

Experiment Log (continued)

[17:53] Stepping pH = 10.58
[18:08] Datapoint id 20 collected
[18:08] Charge balance equation is out by 41.6%
[18:08] pH 10.60 -> 10.80
[18:08] Using cautious pH adjust
[18:08] Dispensed 0.000564 mL of Base (0.5 M KOH)
[18:13] Stepping pH = 10.69
[18:13] Dispensed 0.000541 mL of Base (0.5 M KOH)
[18:18] Stepping pH = 10.77
[18:18] Dispensed 0.000141 mL of Base (0.5 M KOH)
[18:23] Stepping pH = 10.79
[18:23] Dispensed 0.000094 mL of Base (0.5 M KOH)
[18:28] Stepping pH = 10.80
[18:40] Datapoint id 21 collected
[18:40] Charge balance equation is out by 16.4%
[18:40] pH 10.81 -> 11.01
[18:40] Using cautious pH adjust
[18:40] Dispensed 0.000917 mL of Base (0.5 M KOH)
[18:45] Stepping pH = 10.91
[18:45] Dispensed 0.000682 mL of Base (0.5 M KOH)
[18:50] Stepping pH = 10.98
[18:50] Dispensed 0.000259 mL of Base (0.5 M KOH)
[18:55] Stepping pH = 10.99
[18:56] Dispensed 0.000517 mL of Base (0.5 M KOH)
[19:01] Stepping pH = 11.02
[19:12] Datapoint id 22 collected
[19:12] Charge balance equation is out by 28.5%
[19:12] pH 11.03 -> 11.23
[19:12] Using cautious pH adjust
[19:12] Dispensed 0.001529 mL of Base (0.5 M KOH)
[19:17] Stepping pH = 11.12
[19:17] Dispensed 0.001246 mL of Base (0.5 M KOH)
[19:23] Stepping pH = 11.21
[19:23] Dispensed 0.000188 mL of Base (0.5 M KOH)
[19:28] Stepping pH = 11.22
[19:39] Datapoint id 23 collected
[19:39] Charge balance equation is out by 3.4%
[19:39] pH 11.23 -> 11.43
[19:39] Using charge balance adjust
[19:39] Dispensed 0.004868 mL of Base (0.5 M KOH)
[19:56] Datapoint id 24 collected
[19:56] Charge balance equation is out by -2.4%
[19:56] pH 11.42 -> 11.62
[19:56] Using charge balance adjust
[19:56] Dispensed 0.007785 mL of Base (0.5 M KOH)
[20:13] Datapoint id 25 collected
[20:13] Charge balance equation is out by 4.5%
[20:13] pH 11.63 -> 11.83
[20:13] Using charge balance adjust
[20:13] Dispensed 0.012841 mL of Base (0.5 M KOH)
[20:30] Datapoint id 26 collected
[20:30] Charge balance equation is out by -0.8%
[20:30] pH 11.83 -> 12.03
[20:30] Using charge balance adjust
[20:30] Dispensed 0.020790 mL of Base (0.5 M KOH)
[20:47] Datapoint id 27 collected
[20:47] Charge balance equation is out by -5.5%
[20:47] Cleaning up
[20:47] Iterative adjust 12.02 -> 2.00
[20:47] pH 12.02 -> 2.00

Multiset name: **0417936-0002**   Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_ISA_H2O_05_22_18.t3r**

Experiment Log (continued)

[20:47] Stirrer speed set to 20
[20:49] Dispensed 0.100000 mL of Acid (0.5 M HCl)
[20:54] pH 2.10 -> 2.00
[20:55] Dispensed 0.010983 mL of Acid (0.5 M HCl)
[21:00] Holding pH 2.00
[22:04] Dispensed 0.250000 mL of Water (0.15 M KCl)
[22:04] Iterative adjust 1.99 -> 2.00
[22:04] Holding pH 2.00
[22:34] Stirrer speed set to 0
[22:34] Argon flow rate set to 0

Tray Information

Title
Location   A1

UV-metric pKa_0417936-0002   Titration 1 of 1   18E-22004 Points 4 to 36

Results

pKa 1   **4.83**
pKa 2   **8.87**
RMSD   **0.007 0.003 0.007**
Chi squared   **0.0453**
PCA calculated number of pKas   **2**
Average ionic strength   **0.155 M**
Average temperature   **24.9°C**
Analyte concentration range   **61.7 µM to 57.8 µM**

Number of pKas source   **Predicted**
Wavelength clipping   **230.0 nm to 450.0 nm**
pH clipping   **1.466 to 12.552**

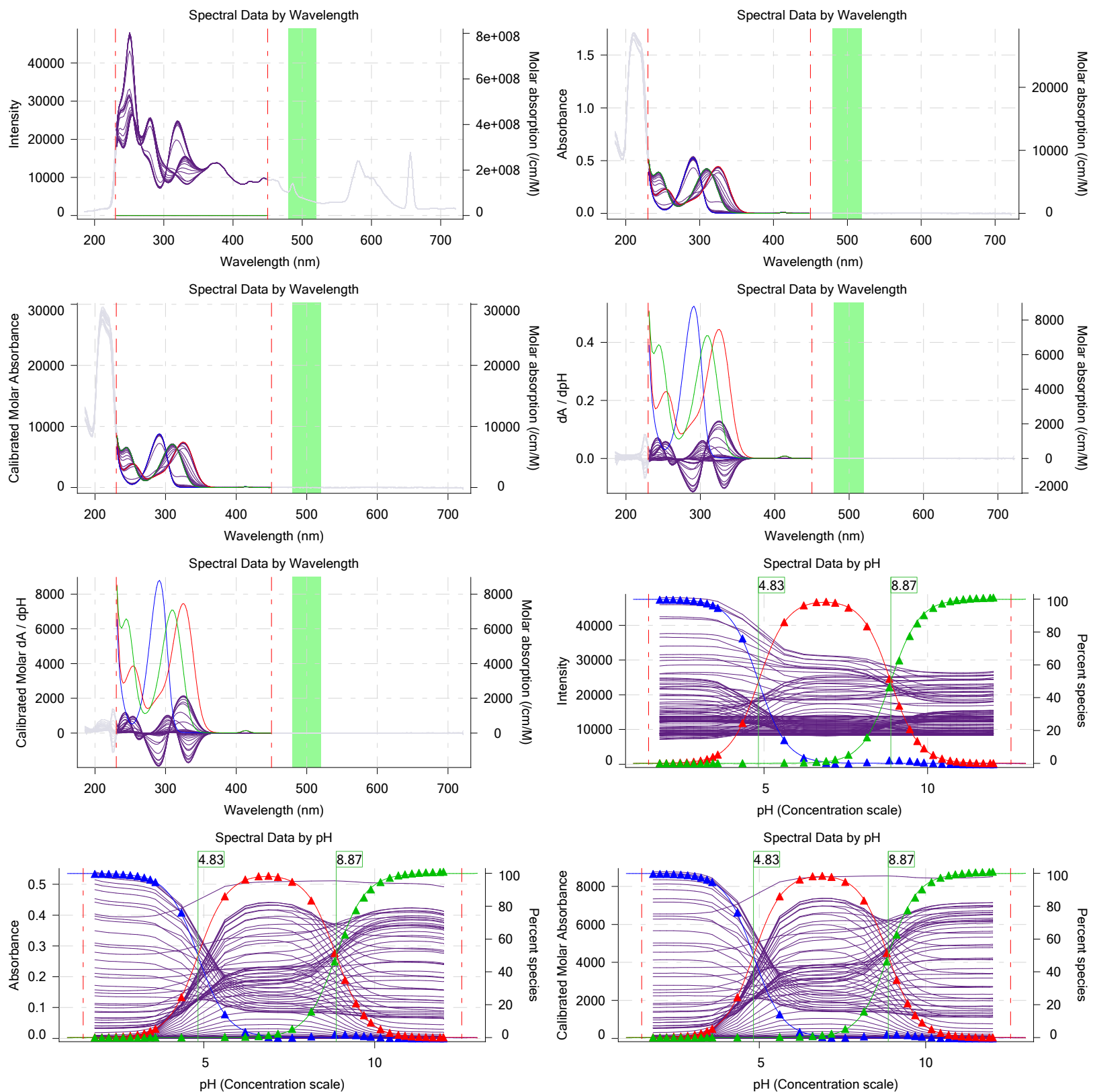## Warnings and errors

Errors   None
Warnings   None

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
Buffer in use	Yes			
Buffer type	Phosphate Buffer			
Assay Medium				
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			

Multiset name: **0417936-0002**   Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
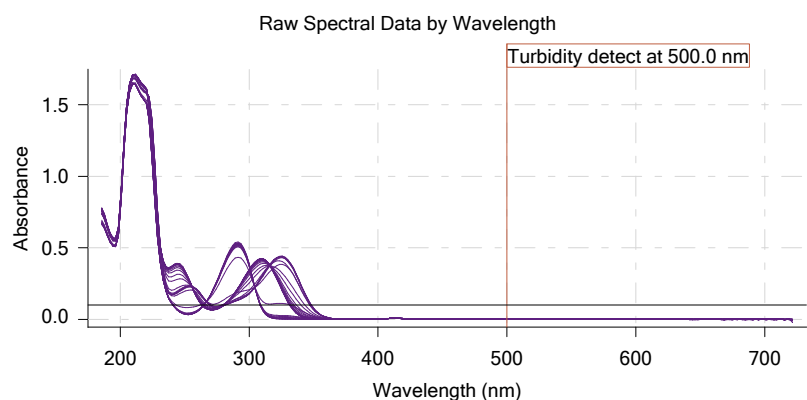Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_ISA_H2O_05_22_18.t3r**

Graphs

UV-metric pKa

Multiset name: **0417936-0002**　　　　　　　　　Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_ISA_H2O_05_22_18.t3r**
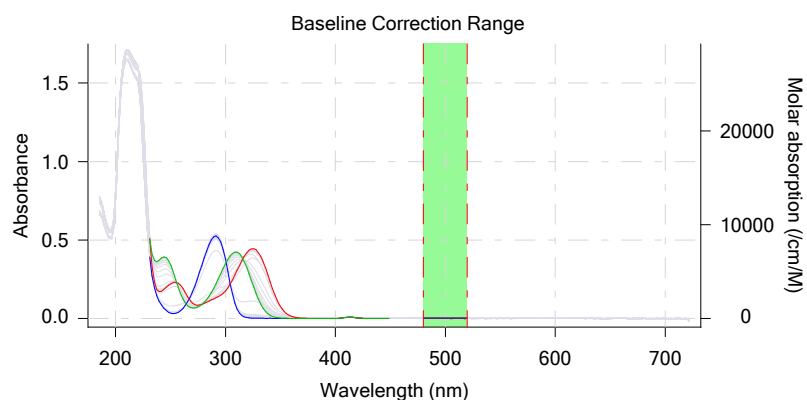
Graphs (continued)

Spectral Data by pH

Spectral Data by pH

PCA Results

Distribution of Species

Molar Absorption Profile

Baseline Correction Range

Raw Spectral Data by Wavelength

UV-metric pKa_0417936-0002　　18E-22004　　Assay 2 of 3

Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
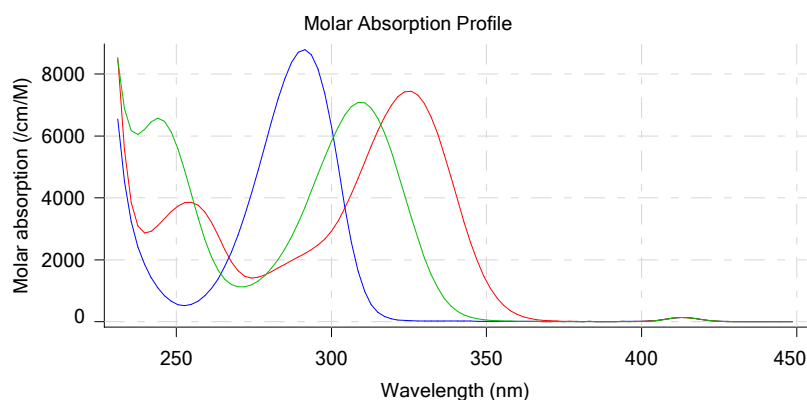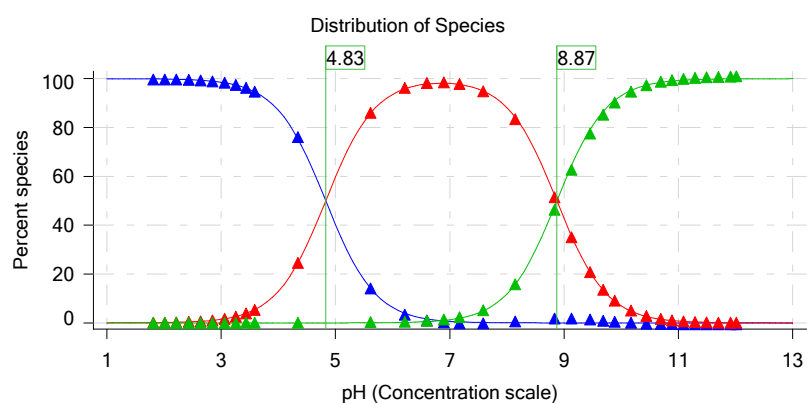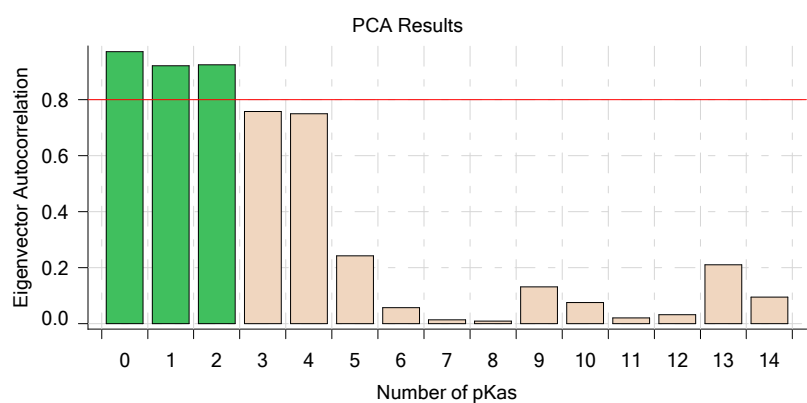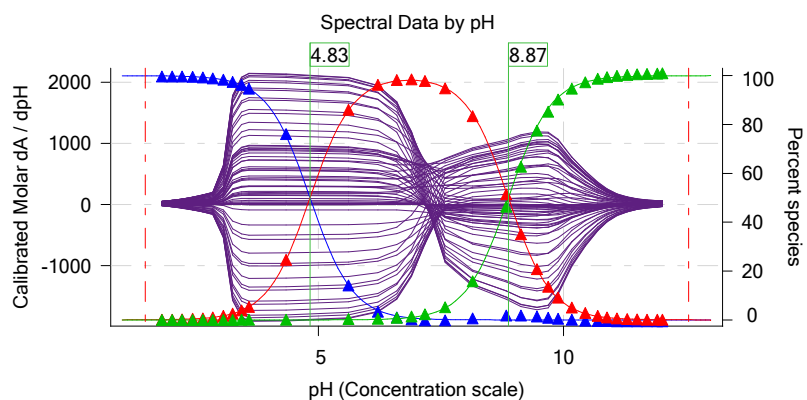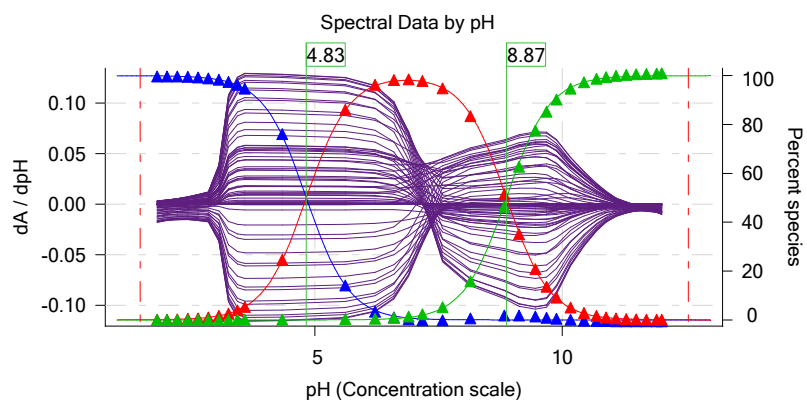Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_ISA_H2O_05_22_18.t3r**

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	Pyridoxine HCl	5/22/2018 9:07:27 AM	User entered value
Sample by	Volume		Default value
Sample volume	0.0020 mL	5/22/2018 9:07:27 AM	User entered value
Solvent	DMSO		Default value
Sample concentration	0.048630 M	5/22/2018 9:07:27 AM	User entered value
Solubility	Unknown		Default value
Molecular weight	205.64	5/22/2018 9:07:35 AM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	2	5/22/2018 9:07:27 AM	User entered value
Sample is a	Ampholyte	5/22/2018 9:07:27 AM	User entered value
pKa 1	4.90	5/22/2018 9:07:27 AM	User entered value
Type	Base	5/22/2018 9:07:27 AM	User entered value
pKa 2	8.80	5/22/2018 9:07:27 AM	User entered value
Type	Acid	5/22/2018 9:07:27 AM	User entered value
logp (XH2 +)	-10.00		Default value
logP (neutral XH)	-10.00	5/22/2018 9:07:27 AM	User entered value
logP (X -)	-10.00		Default value
Stoichiometry	1.00000		Default value
Aprotic counterion name	Chloride		From standards.xml file
Stoichiometry	1.00		From standards.xml file
Charge per counterion	-1		From standards.xml file

Events

Time	Event	Water	Acid	Base	Buffer	pH	dpH/dt	pH R-squared	pH SD
3:24.7	Dark spectrum								
3:26.3	Reference spectrum								
3:54.0	Volume reset due to vial change								
5:24.4	Initial pH = 7.03								
6:27.6	Data point 4	1.50000 mL	0.04986 mL	0.00000 mL	0.02500 mL	1.966	-0.00757	0.56671	0.000
6:56.3	Data point 5	1.50000 mL	0.04986 mL	0.01804 mL	0.02500 mL	2.164	0.00943	0.62450	0.000
7:13.2	Data point 6	1.50000 mL	0.04986 mL	0.02944 mL	0.02500 mL	2.360	-0.00099	0.01699	0.000
7:30.1	Data point 7	1.50000 mL	0.04986 mL	0.03669 mL	0.02500 mL	2.571	-0.00281	0.05908	0.000
7:46.9	Data point 8	1.50000 mL	0.04986 mL	0.04111 mL	0.02500 mL	2.777	0.01674	0.88270	0.000
8:03.6	Data point 9	1.50000 mL	0.04986 mL	0.04381 mL	0.02500 mL	2.981	0.02333	0.92685	0.001
8:20.3	Data point 10	1.50000 mL	0.04986 mL	0.04548 mL	0.02500 mL	3.192	0.01561	0.92316	0.000
8:37.0	Data point 11	1.50000 mL	0.04986 mL	0.04652 mL	0.02500 mL	3.382	0.01511	0.89366	0.000
8:53.7	Data point 12	1.50000 mL	0.04986 mL	0.04718 mL	0.02500 mL	3.561	0.02978	0.98482	0.001
9:10.4	Data point 13	1.50000 mL	0.04986 mL	0.04760 mL	0.02500 mL	3.710	0.05023	0.98647	0.002
9:37.4	Data point 14	1.50000 mL	0.04986 mL	0.04873 mL	0.02500 mL	4.460	0.09744	0.98898	0.004
10:26.4	Data point 15	1.50000 mL	0.04986 mL	0.04915 mL	0.02500 mL	5.719	0.09590	0.94209	0.004
11:29.9	Data point 16	1.50000 mL	0.04986 mL	0.04944 mL	0.02500 mL	6.315	0.09835	0.99059	0.004
12:05.7	Data point 17	1.50000 mL	0.04986 mL	0.04965 mL	0.02500 mL	6.697	0.09733	0.95539	0.004
12:40.6	Data point 18	1.50000 mL	0.04986 mL	0.04981 mL	0.02500 mL	6.990	0.09845	0.98806	0.004
13:14.5	Data point 19	1.50000 mL	0.04986 mL	0.04993 mL	0.02500 mL	7.264	0.09988	0.99331	0.004
13:59.0	Data point 20	1.50000 mL	0.04986 mL	0.05005 mL	0.02500 mL	7.671	0.09246	0.95444	0.004
14:57.4	Data point 21	1.50000 mL	0.04986 mL	0.05016 mL	0.02500 mL	8.226	0.09551	0.91125	0.004
15:49.3	Data point 22	1.50000 mL	0.04986 mL	0.05033 mL	0.02500 mL	8.907	0.09884	0.99191	0.004
16:29.6	Data point 23	1.50000 mL	0.04986 mL	0.05045 mL	0.02500 mL	9.204	0.10049	0.98916	0.004
16:59.7	Data point 24	1.50000 mL	0.04986 mL	0.05061 mL	0.02500 mL	9.525	0.09602	0.98217	0.004
17:24.8	Data point 25	1.50000 mL	0.04986 mL	0.05078 mL	0.02500 mL	9.751	0.09352	0.96911	0.004
17:47.1	Data point 26	1.50000 mL	0.04986 mL	0.05096 mL	0.02500 mL	9.953	0.07957	0.96208	0.004
18:03.9	Data point 27	1.50000 mL	0.04986 mL	0.05125 mL	0.02500 mL	10.234	0.01091	0.87155	0.000
18:30.9	Data point 28	1.50000 mL	0.04986 mL	0.05181 mL	0.02500 mL	10.504	-0.00487	0.70957	0.000
18:47.7	Data point 29	1.50000 mL	0.04986 mL	0.05273 mL	0.02500 mL	10.751	0.00034	0.00611	0.000
19:15.8	Data point 30	1.50000 mL	0.04986 mL	0.05430 mL	0.02500 mL	10.945	-0.00631	0.51904	0.000
19:32.5	Data point 31	1.50000 mL	0.04986 mL	0.05684 mL	0.02500 mL	11.143	0.00276	0.28131	0.000
19:49.4	Data point 32	1.50000 mL	0.04986 mL	0.06087 mL	0.02500 mL	11.345	-0.00336	0.25554	0.000

Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_ISA_H2O_05_22_18.t3r**

Events (continued)

Time	Event	Water	Acid	Base	Buffer	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
20:06.3	Data point 33	1.50000 mL	0.04986 mL	0.06738 mL	0.02500 mL	11.544	0.00542	0.72199	0.00032	10.0 s
20:23.3	Data point 34	1.50000 mL	0.04986 mL	0.07780 mL	0.02500 mL	11.747	0.00335	0.20625	0.00036	10.0 s
20:40.4	Data point 35	1.50000 mL	0.04986 mL	0.09473 mL	0.02500 mL	11.951	0.01060	0.78631	0.00059	10.0 s
20:57.3	Data point 36	1.50000 mL	0.04986 mL	0.10687 mL	0.02500 mL	12.052	0.00724	0.77837	0.00040	10.0 s
22:56.3	Assay volumes	1.75000 mL	0.16853 mL	0.10687 mL	0.02500 mL					

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				
Analyst name	Dorothy Levorse			
Separate reference vial	Yes			
Standard Experiment Settings				
Number of titrations	1			
Minimum pH	2.000			
Maximum pH	12.000			
pH step between points of	0.200			
Minimum titrant addition	0.00002 mL			
Maximum titrant addition	0.10000 mL			
Argon flow rate	100%			
Start titration using	Cautious pH adjust			
Advanced General Settings				
Detect turbidity using	Spectrometer			
Monitor at a wavelength of	500.0 nm			
Absorbance threshold of	0.100			
Collect turbidity sensor data	No			
Stir after titrant addition for	5 seconds			
For titrant addition, stir at	15%			
Titrant Pre-Dose				
Titrant pre-dose	None			
Assay Medium				
Cosolvent in use	No			
ISA water volume	1.50 mL			
Water added	Automatic			
After water addition, stir for	5 seconds			
At a speed of	15%			
Buffer in use	Yes			
Buffer type	Phosphate Buffer			
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			
After medium addition, stir for	5 seconds			
Sample Sonication				
Sonicate	No			
Sample Dissolution				
Perform a dissolution stage	No			
Carbonate purge				
Perform a carbonate purge	No			
Temperature Control				
Wait for temperature	Yes			
Required start temperature	25.0°C			
Acceptable deviation	0.5°C			
Time to wait	60 seconds			
Stir speed of	15%			
Titration 1				
Titrate from	Low to high pH			
Adjust to start pH	Yes			
After pH adjust stir for	10 seconds			
Data Point Stability				
Stir during data point collection	Yes			

Multiset name: **0417936-0002**　　　　　　　　　　Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_ISA_H2O_05_22_18.t3r**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
For point collection, stir at	15%			
Delay before data point collection	0 seconds			
Number of points to average	20 points			
Time interval between points	0.50 seconds			
Required maximum standard deviation	0.00500 dpH/dt			
Stability timeout after	60 seconds			
Experiment cleanup				
Adjust pH to cleanup	To start pH			
And then stir for	60 seconds			
For cleaning, stir at	20%			
Then add water volume	0.25 mL			
And then stir for	30 seconds			

Calibration Settings

Setting	Value	Date/Time changed	Imported from
Four-Plus alpha	0.160	5/22/2018 10:11:10 AM	C:\Sirius_T3\18E-21006_Blank standardisation.t3r
Four-Plus S	0.9904	5/22/2018 10:11:10 AM	C:\Sirius_T3\18E-21006_Blank standardisation.t3r
Four-Plus jH	1.0	5/22/2018 10:11:10 AM	C:\Sirius_T3\18E-21006_Blank standardisation.t3r
Four-Plus jOH	-0.5	5/22/2018 10:11:10 AM	C:\Sirius_T3\18E-21006_Blank standardisation.t3r
Base concentration factor	1.012	5/22/2018 10:11:10 AM	C:\Sirius_T3\KOH18D10.t3r
Acid concentration factor	1.011	5/22/2018 10:11:10 AM	C:\Sirius_T3\18E-21006_Blank standardisation.t3r

Instrument Settings

Setting	Value	Batch Id	Install date
Instrument owner	Merck		
Instrument ID	T311053		
Instrument type	T3 Simulator		
Software version	1.1.3.0		
Dispenser module		T3DM1100253	3/31/2009 6:24:52 AM
Dispenser 0	Water		3/31/2009 6:25:05 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Water (0.15 M KCl)	2-6-18	5/15/2018 2:12:22 PM
Dispenser 2	Acid		3/31/2009 6:25:11 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Acid (0.5 M HCl)	3-22-18	5/15/2018 2:12:48 PM
Dispenser 1	Base		3/31/2009 6:25:21 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Base (0.5 M KOH)	3-22-18	5/15/2018 2:12:34 PM
Dispenser 5	Cosolvent		3/31/2009 6:26:24 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Distribution valve 5	Distribution Valve		3/31/2009 6:28:19 AM
Firmware version	1.1.3		
Port A	Methanol (80%, 0.15 M KCl)	2-8-18	5/15/2018 2:14:14 PM
Port B	Cyclohexane		4/10/2018 8:40:51 AM
Port C	MeCN (50%, 0.15 M KCl)	4-16-18	5/15/2018 2:14:20 PM
Dispenser 3	Buffer		8/3/2010 6:05:16 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Dodecane	1-31-2018	5/15/2018 2:12:54 PM
Dispenser 6	Octanol		10/22/2010 11:52:43 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Octanol	1-31-2018	4/9/2018 9:14:11 AM
Titrator		T3TM1100153	3/31/2009 6:24:17 AM

Multiset name: **0417936-0002**   Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_ISA_H2O_05_22_18.t3r**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Horizontal axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Probe I/O firmware version	1.1.1		
Electrode	T3 Electrode	T3E0769	8/15/2017 10:21:54 AM
E0 calibration	-9.08 mV		5/22/2018 10:11:34 AM
Filling solution	3M KCl	KCL095	5/21/2018 8:57:01 AM
Liquids			
Wash 1	50% IPA:50% Water		5/22/2018 8:38:15 AM
Wash 2	0.5% Trition X-100 in H20		5/22/2018 8:38:18 AM
Buffer position 1	pH7 Wash		5/22/2018 8:38:22 AM
Buffer position 2	pH 7		5/22/2018 8:38:25 AM
Storage position			5/22/2018 8:38:32 AM
Wash water	3.8e+003 mL	5-15-18	5/15/2018 2:11:48 PM
Waste	6.7e+003 mL		3/19/2018 10:48:12 AM
Temperature controller			8/5/2010 7:35:13 AM
Turbidity detector			3/31/2009 6:24:45 AM
Spectrometer		072390	11/23/2010 12:22:28 PM
Dip probe		11086	
Wavelength coefficient A0	185.563		
Wavelength coefficient A1	2.17439		
Wavelength coefficient A2	-0.000285622		
Total lamp lit time	897:26:49		11/23/2010 12:22:28 PM
Calibrated on	5/21/2018 2:44:22 PM		
Integration time	19		
Scans averaged	10		
Autoloader		T3AL1100237	11/10/2015 10:34:13 AM
Left-right axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Front-back axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Configuration			
Alternate titration position	Titration position		
Alternate reference position	Reference position		
Maximum standard vial volume	3.50 mL		
Maximum alternate vial volume	25.00 mL		
Automatic action idle period	5 minute(s)		
Titrant tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		
Flowing wash stir speed	30%		
Solvent wash stir duration	5 s		
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		
E0 calibration reading stir speed	0%		
Spectrometer calibration stir duration	5 s		
Spectrometer calibration stir speed	30%		
Spectrometer calibration wash pump volume	20.0 mL		
Spectrometer calibration wash stir duration	5 s		
Spectrometer calibration wash stir speed	30%		

Multiset name: **0417936-0002**   Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_ISA_H2O_05_22_18.t3r**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Overhead dispense height	10000		

Refinement Settings

Setting	Value	Default value
Turbidity detection method	Spectrometer	Spectrometer
Turbidity wavelength to assess	500.0 nm	500.0 nm
Turbidity maximum absorbance	0.100	0.100
Turbidity probe threshold	50.00	50.00
Exclude turbid points	Yes	Yes
Low intensity warning threshold	100	100
Minimum absorbance change threshold	0.100	0.100
Eigenvector autocorrelation threshold	0.80	0.80
Maximum RMSD severe warning	0.250	0.250
Maximum RMSD warning	0.050	0.050

Experiment Log

[2:06] Air gap created for Water (0.15 M KCl)
[2:06] Air gap created for Acid (0.5 M HCl)
[2:07] Air gap created for Base (0.5 M KOH)
[2:07] Air gap released for Water (0.15 M KCl)
[2:11] Titrator arm moved to Reference position
[2:11] Argon flow rate set to 100
[2:11] Preparing reference vial
[2:11] Automatically add 1.50000 mL of water
[2:37] Dispensed 1.500000 mL of Water (0.15 M KCl)
[2:37] Stirrer speed set to 15
[2:47] Iterative adjust 7.63 -> 2.00
[2:47] pH 7.63 -> 2.00
[2:48] Air gap released for Acid (0.5 M HCl)
[2:49] Dispensed 0.043744 mL of Acid (0.5 M HCl)
[2:54] pH 2.06 -> 2.00
[2:55] Dispensed 0.006115 mL of Acid (0.5 M HCl)
[3:00] Stirrer speed set to 0
[3:03] Titrator arm moved over Reference position
[3:04] Air gap created for Water (0.15 M KCl)
[3:04] Air gap created for Acid (0.5 M HCl)
[3:08] Titrator arm moved to Reference position
[3:08] Air gap released for Water (0.15 M KCl)
[3:08] Stirrer speed set to 15
[3:23] Stirrer speed set to 0
[3:25] Dark scan collected
[3:26] Reference scan collected
[3:54] Probes washed
[3:54] Volume reset due to vial change
[4:03] Titrator arm moved to Titration position
[4:03] Preparing sample vial
[4:03] Automatically add 1.50000 mL of water
[5:14] Dispensed 1.500000 mL of Water (0.15 M KCl)
[5:14] Stirrer speed set to 15
[5:24] Initial pH = 7.03
[5:24] Adding reagent volumes used in reference
[5:24]   Adding acid volume of 0.0498589
[5:26] Air gap released for Acid (0.5 M HCl)
[5:27] Dispensed 0.049859 mL of Acid (0.5 M HCl)
[6:39] Datapoint id 4 collected
[6:39] pH 1.97 -> 2.17
[6:39] Using cautious pH adjust
[6:40] Air gap released for Base (0.5 M KOH)

Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_ISA_H2O_05_22_18.t3r**

Experiment Log (continued)

[6:41] Dispensed 0.009219 mL of Base (0.5 M KOH)
[6:46] Stepping pH = 2.05
[6:46] Dispensed 0.006938 mL of Base (0.5 M KOH)
[6:51] Stepping pH = 2.14
[6:51] Dispensed 0.001881 mL of Base (0.5 M KOH)
[6:56] Stepping pH = 2.16
[7:08] Datapoint id 5 collected
[7:08] Charge balance equation is out by 1.9%
[7:08] pH 2.16 -> 2.36
[7:08] Using charge balance adjust
[7:08] Dispensed 0.011406 mL of Base (0.5 M KOH)
[7:25] Datapoint id 6 collected
[7:25] Charge balance equation is out by -1.8%
[7:25] pH 2.36 -> 2.56
[7:25] Using charge balance adjust
[7:25] Dispensed 0.007244 mL of Base (0.5 M KOH)
[7:42] Datapoint id 7 collected
[7:42] Charge balance equation is out by 5.5%
[7:42] pH 2.57 -> 2.77
[7:42] Using charge balance adjust
[7:42] Dispensed 0.004421 mL of Base (0.5 M KOH)
[7:58] Datapoint id 8 collected
[7:58] Charge balance equation is out by 2.7%
[7:58] pH 2.78 -> 2.98
[7:58] Using charge balance adjust
[7:59] Dispensed 0.002705 mL of Base (0.5 M KOH)
[8:15] Datapoint id 9 collected
[8:15] Charge balance equation is out by 2.1%
[8:15] pH 2.98 -> 3.18
[8:15] Using charge balance adjust
[8:15] Dispensed 0.001670 mL of Base (0.5 M KOH)
[8:32] Datapoint id 10 collected
[8:32] Charge balance equation is out by 5.4%
[8:32] pH 3.19 -> 3.39
[8:32] Using charge balance adjust
[8:32] Dispensed 0.001035 mL of Base (0.5 M KOH)
[8:49] Datapoint id 11 collected
[8:49] Charge balance equation is out by -5.0%
[8:49] pH 3.38 -> 3.58
[8:49] Using charge balance adjust
[8:49] Dispensed 0.000659 mL of Base (0.5 M KOH)
[9:05] Datapoint id 12 collected
[9:05] Charge balance equation is out by -10.4%
[9:05] pH 3.56 -> 3.76
[9:05] Using charge balance adjust
[9:05] Dispensed 0.000423 mL of Base (0.5 M KOH)
[9:22] Datapoint id 13 collected
[9:22] Charge balance equation is out by -25.6%
[9:22] pH 3.71 -> 3.91
[9:22] Using cautious pH adjust
[9:22] Dispensed 0.000165 mL of Base (0.5 M KOH)
[9:27] Stepping pH = 3.73
[9:27] Dispensed 0.000423 mL of Base (0.5 M KOH)
[9:32] Stepping pH = 3.78
[9:32] Dispensed 0.000541 mL of Base (0.5 M KOH)
[9:38] Stepping pH = 4.40
[10:11] Datapoint id 14 collected
[10:11] Charge balance equation is out by 251.4%
[10:11] pH 4.46 -> 4.66
[10:11] Using cautious pH adjust

Multiset name: **0417936-0002**   Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_ISA_H2O_05_22_18.t3r**

Experiment Log (continued)

[10:11] Dispensed 0.000024 mL of Base (0.5 M KOH)
[10:16] Stepping pH = 4.48
[10:16] Dispensed 0.000094 mL of Base (0.5 M KOH)
[10:21] Stepping pH = 4.48
[10:21] Dispensed 0.000306 mL of Base (0.5 M KOH)
[10:26] Stepping pH = 5.57
[11:14] Datapoint id 15 collected
[11:14] Charge balance equation is out by 485.2%
[11:14] pH 5.72 -> 5.92
[11:14] Using cautious pH adjust
[11:15] Dispensed 0.000024 mL of Base (0.5 M KOH)
[11:20] Stepping pH = 5.73
[11:20] Dispensed 0.000071 mL of Base (0.5 M KOH)
[11:25] Stepping pH = 5.73
[11:25] Dispensed 0.000188 mL of Base (0.5 M KOH)
[11:30] Stepping pH = 6.26
[11:50] Datapoint id 16 collected
[11:50] Charge balance equation is out by 517.7%
[11:50] pH 6.32 -> 6.52
[11:50] Using cautious pH adjust
[11:50] Dispensed 0.000024 mL of Base (0.5 M KOH)
[11:56] Stepping pH = 6.33
[11:56] Dispensed 0.000047 mL of Base (0.5 M KOH)
[12:01] Stepping pH = 6.35
[12:01] Dispensed 0.000141 mL of Base (0.5 M KOH)
[12:06] Stepping pH = 6.68
[12:25] Datapoint id 17 collected
[12:25] Charge balance equation is out by 458.4%
[12:25] pH 6.70 -> 6.90
[12:25] Using cautious pH adjust
[12:25] Dispensed 0.000024 mL of Base (0.5 M KOH)
[12:30] Stepping pH = 6.71
[12:30] Dispensed 0.000047 mL of Base (0.5 M KOH)
[12:36] Stepping pH = 6.74
[12:36] Dispensed 0.000094 mL of Base (0.5 M KOH)
[12:41] Stepping pH = 6.94
[12:59] Datapoint id 18 collected
[12:59] Charge balance equation is out by 427.0%
[12:59] pH 6.99 -> 7.19
[12:59] Using cautious pH adjust
[12:59] Dispensed 0.000024 mL of Base (0.5 M KOH)
[13:04] Stepping pH = 7.01
[13:04] Dispensed 0.000024 mL of Base (0.5 M KOH)
[13:09] Stepping pH = 7.03
[13:10] Dispensed 0.000071 mL of Base (0.5 M KOH)
[13:15] Stepping pH = 7.19
[13:39] Datapoint id 19 collected
[13:39] Charge balance equation is out by 473.6%
[13:39] pH 7.26 -> 7.46
[13:39] Using cautious pH adjust
[13:39] Dispensed 0.000024 mL of Base (0.5 M KOH)
[13:44] Stepping pH = 7.28
[13:44] Dispensed 0.000024 mL of Base (0.5 M KOH)
[13:49] Stepping pH = 7.30
[13:49] Dispensed 0.000047 mL of Base (0.5 M KOH)
[13:54] Stepping pH = 7.41
[13:54] Dispensed 0.000024 mL of Base (0.5 M KOH)
[13:59] Stepping pH = 7.53
[14:37] Datapoint id 20 collected
[14:37] Charge balance equation is out by 702.4%

Multiset name: **0417936-0002**   Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_ISA_H2O_05_22_18.t3r**

Experiment Log (continued)

[14:37] pH 7.67 -> 7.87
[14:37] Using cautious pH adjust
[14:37] Dispensed 0.000024 mL of Base (0.5 M KOH)
[14:42] Stepping pH = 7.68
[14:42] Dispensed 0.000024 mL of Base (0.5 M KOH)
[14:47] Stepping pH = 7.68
[14:47] Dispensed 0.000047 mL of Base (0.5 M KOH)
[14:52] Stepping pH = 7.85
[14:53] Dispensed 0.000024 mL of Base (0.5 M KOH)
[14:58] Stepping pH = 8.02
[15:34] Datapoint id 21 collected
[15:34] Charge balance equation is out by 822.7%
[15:34] pH 8.23 -> 8.43
[15:34] Using cautious pH adjust
[15:34] Dispensed 0.000024 mL of Base (0.5 M KOH)
[15:39] Stepping pH = 8.23
[15:39] Dispensed 0.000047 mL of Base (0.5 M KOH)
[15:44] Stepping pH = 8.25
[15:44] Dispensed 0.000094 mL of Base (0.5 M KOH)
[15:49] Stepping pH = 8.79
[16:19] Datapoint id 22 collected
[16:19] Charge balance equation is out by 532.4%
[16:19] pH 8.91 -> 9.11
[16:19] Using cautious pH adjust
[16:19] Dispensed 0.000024 mL of Base (0.5 M KOH)
[16:24] Stepping pH = 8.92
[16:25] Dispensed 0.000094 mL of Base (0.5 M KOH)
[16:30] Stepping pH = 9.15
[16:50] Datapoint id 23 collected
[16:50] Charge balance equation is out by 92.6%
[16:50] pH 9.20 -> 9.40
[16:50] Using cautious pH adjust
[16:50] Dispensed 0.000047 mL of Base (0.5 M KOH)
[16:55] Stepping pH = 9.23
[16:55] Dispensed 0.000118 mL of Base (0.5 M KOH)
[17:00] Stepping pH = 9.50
[17:15] Datapoint id 24 collected
[17:15] Charge balance equation is out by 82.9%
[17:15] pH 9.53 -> 9.73
[17:15] Using cautious pH adjust
[17:15] Dispensed 0.000071 mL of Base (0.5 M KOH)
[17:20] Stepping pH = 9.58
[17:20] Dispensed 0.000094 mL of Base (0.5 M KOH)
[17:25] Stepping pH = 9.74
[17:37] Datapoint id 25 collected
[17:37] Charge balance equation is out by 22.7%
[17:37] pH 9.75 -> 9.95
[17:37] Using cautious pH adjust
[17:37] Dispensed 0.000094 mL of Base (0.5 M KOH)
[17:42] Stepping pH = 9.84
[17:42] Dispensed 0.000094 mL of Base (0.5 M KOH)
[17:47] Stepping pH = 9.94
[17:59] Datapoint id 26 collected
[17:59] Charge balance equation is out by 6.5%
[17:59] pH 9.95 -> 10.15
[17:59] Using charge balance adjust
[17:59] Dispensed 0.000282 mL of Base (0.5 M KOH)
[18:16] Datapoint id 27 collected
[18:16] Charge balance equation is out by 40.3%
[18:16] pH 10.23 -> 10.43

Multiset name: **0417936-0002**   Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_ISA_H2O_05_22_18.t3r**

Experiment Log (continued)

[18:16] Using cautious pH adjust
[18:16] Dispensed 0.000259 mL of Base (0.5 M KOH)
[18:21] Stepping pH = 10.39
[18:21] Dispensed 0.000071 mL of Base (0.5 M KOH)
[18:26] Stepping pH = 10.39
[18:26] Dispensed 0.000235 mL of Base (0.5 M KOH)
[18:31] Stepping pH = 10.50
[18:43] Datapoint id 28 collected
[18:43] Charge balance equation is out by 10.6%
[18:43] pH 10.50 -> 10.70
[18:43] Using charge balance adjust
[18:43] Dispensed 0.000917 mL of Base (0.5 M KOH)
[19:00] Datapoint id 29 collected
[19:00] Charge balance equation is out by 23.7%
[19:00] pH 10.75 -> 10.95
[19:00] Using cautious pH adjust
[19:00] Dispensed 0.000800 mL of Base (0.5 M KOH)
[19:06] Stepping pH = 10.86
[19:06] Dispensed 0.000541 mL of Base (0.5 M KOH)
[19:11] Stepping pH = 10.92
[19:11] Dispensed 0.000235 mL of Base (0.5 M KOH)
[19:16] Stepping pH = 10.94
[19:27] Datapoint id 30 collected
[19:27] Charge balance equation is out by 2.1%
[19:27] pH 10.94 -> 11.14
[19:27] Using charge balance adjust
[19:28] Dispensed 0.002540 mL of Base (0.5 M KOH)
[19:44] Datapoint id 31 collected
[19:44] Charge balance equation is out by -0.6%
[19:44] pH 11.14 -> 11.34
[19:44] Using charge balance adjust
[19:44] Dispensed 0.004022 mL of Base (0.5 M KOH)
[20:01] Datapoint id 32 collected
[20:01] Charge balance equation is out by 1.1%
[20:01] pH 11.35 -> 11.55
[20:01] Using charge balance adjust
[20:01] Dispensed 0.006515 mL of Base (0.5 M KOH)
[20:18] Datapoint id 33 collected
[20:18] Charge balance equation is out by -0.5%
[20:18] pH 11.54 -> 11.74
[20:18] Using charge balance adjust
[20:18] Dispensed 0.010419 mL of Base (0.5 M KOH)
[20:35] Datapoint id 34 collected
[20:35] Charge balance equation is out by 1.1%
[20:35] pH 11.75 -> 11.95
[20:35] Using charge balance adjust
[20:35] Dispensed 0.016933 mL of Base (0.5 M KOH)
[20:52] Datapoint id 35 collected
[20:52] Charge balance equation is out by 2.3%
[20:52] pH 11.95 -> 12.05
[20:52] Using charge balance adjust
[20:52] Dispensed 0.012135 mL of Base (0.5 M KOH)
[21:09] Datapoint id 36 collected
[21:09] Charge balance equation is out by -49.6%
[21:09] Cleaning up
[21:09] Iterative adjust 12.05 -> 2.00
[21:09] pH 12.05 -> 2.00
[21:09] Stirrer speed set to 20
[21:11] Dispensed 0.100000 mL of Acid (0.5 M HCl)
[21:16] pH 2.19 -> 2.00

Multiset name: **0417936-0002**   Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_ISA_H2O_05_22_18.t3r**

Experiment Log (continued)

[21:17] Dispensed 0.018674 mL of Acid (0.5 M HCl)
[21:22] Holding pH 2.00
[22:26] Dispensed 0.250000 mL of Water (0.15 M KCl)
[22:26] Iterative adjust 2.01 -> 2.00
[22:26] Holding pH 2.00
[22:56] Stirrer speed set to 0
[22:56] Argon flow rate set to 0

Tray Information

Title
Location   A3

UV-metric pKa_0417936-0002   Titration 1 of 1   18E-22010 Points 4 to 38

Results

pKa 1   **4.84**
pKa 2   **8.86**
RMSD   **0.006 0.002 0.006**
Chi squared   **0.0383**
PCA calculated number of pKas **2**
Average ionic strength   **0.155 M**
Average temperature   **24.9°C**
Analyte concentration range   **61.7 µM to 58.0 µM**

Number of pKas source   **Predicted**
Wavelength clipping   **230.0 nm to 450.0 nm**
pH clipping   **1.463 to 12.502**
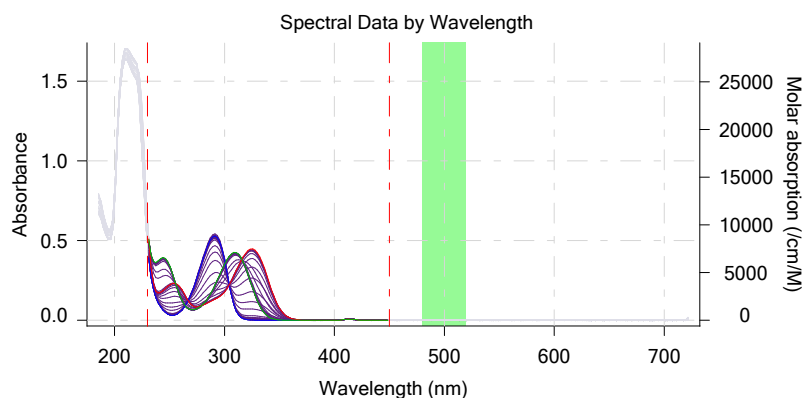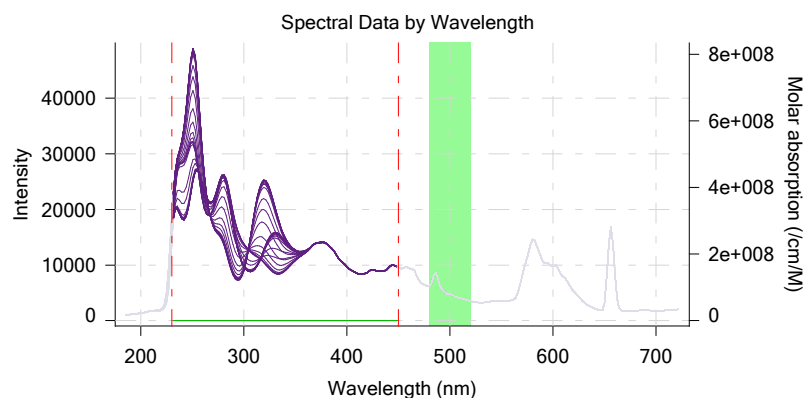
Warnings and errors

Errors   None
Warnings   None

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
Buffer in use	Yes			
Buffer type	Phosphate Buffer			
Assay Medium				
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			

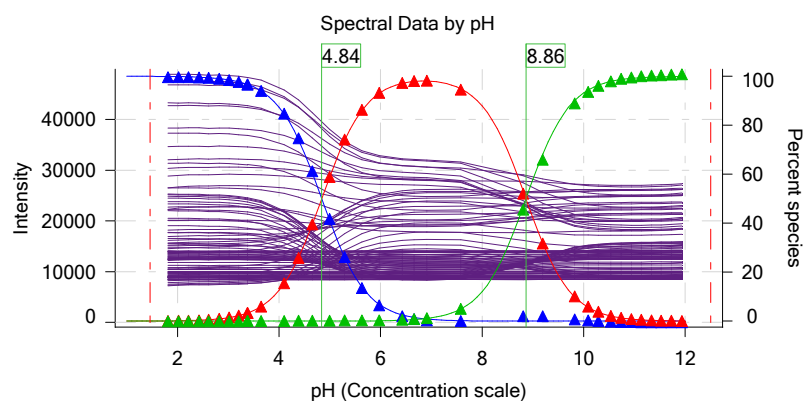## Graphs

UV-metric pKa

Multiset name: **0417936-0002**   Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_ISA_H2O_05_22_18.t3r**

Graphs (continued)

Spectral Data by Wavelength

Spectral Data by Wavelength

Spectral Data by Wavelength

Spectral Data by pH

Spectral Data by pH

Spectral Data by pH

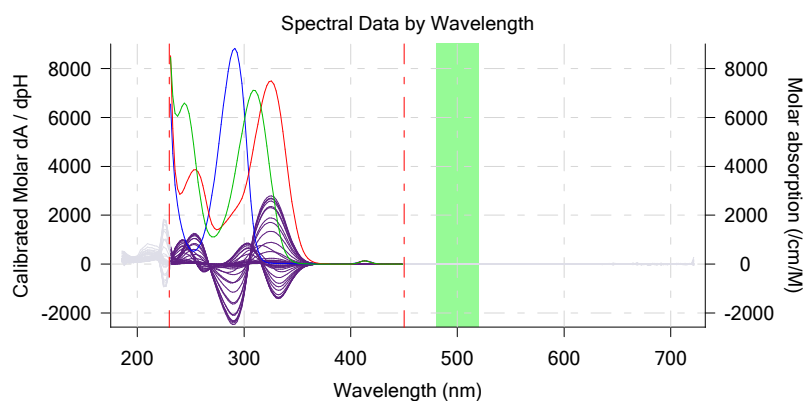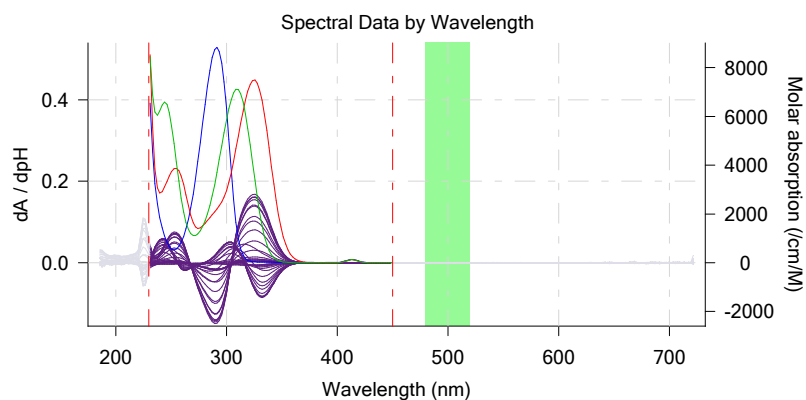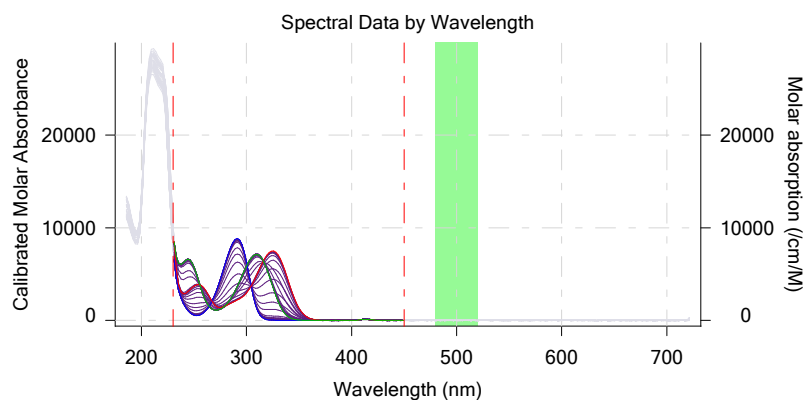Spectral Data by pH

Spectral Data by pH

Multiset name: **0417936-0002**   Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_ISA_H2O_05_22_18.t3r**
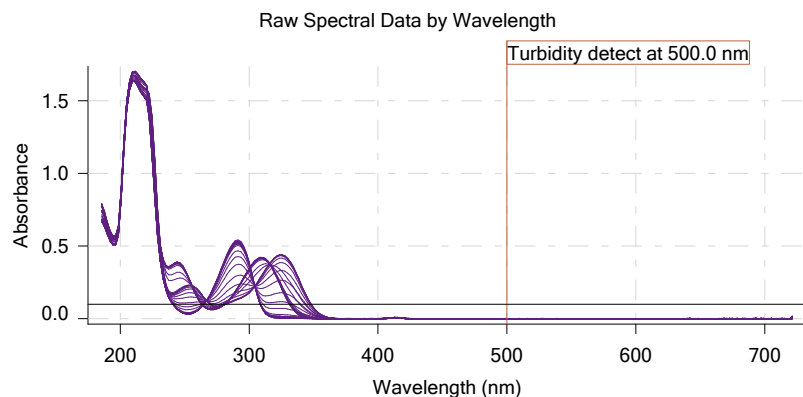
Graphs (continued)

PCA Results

Distribution of Species

Molar Absorption Profile

Baseline Correction Range

Raw Spectral Data by Wavelength

Turbidity detect at 500.0 nm
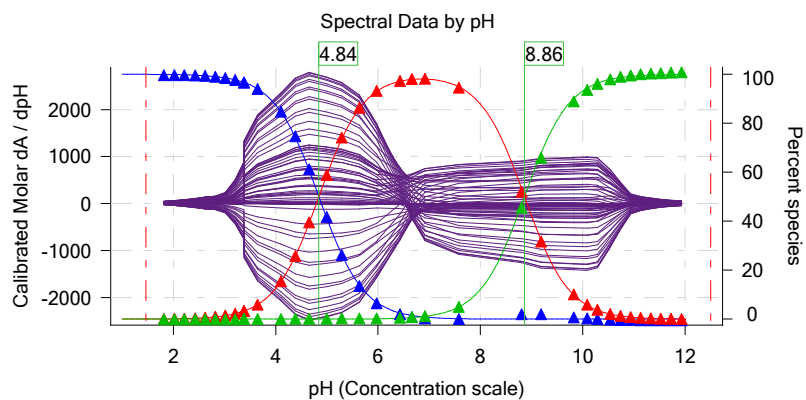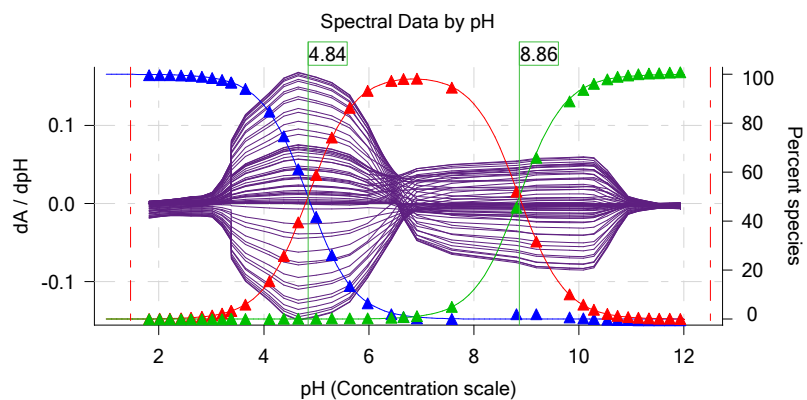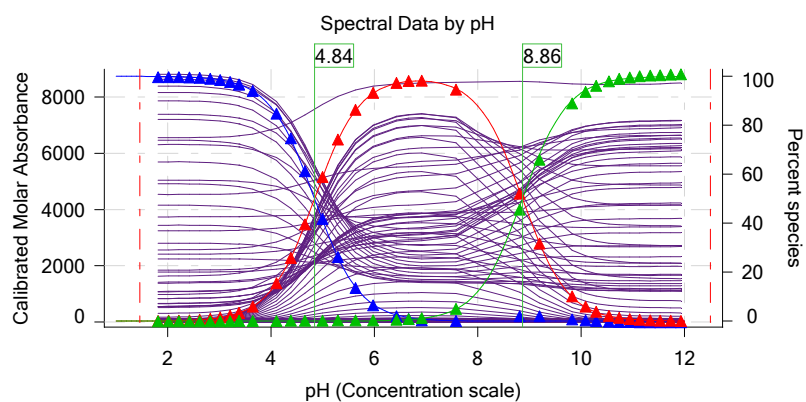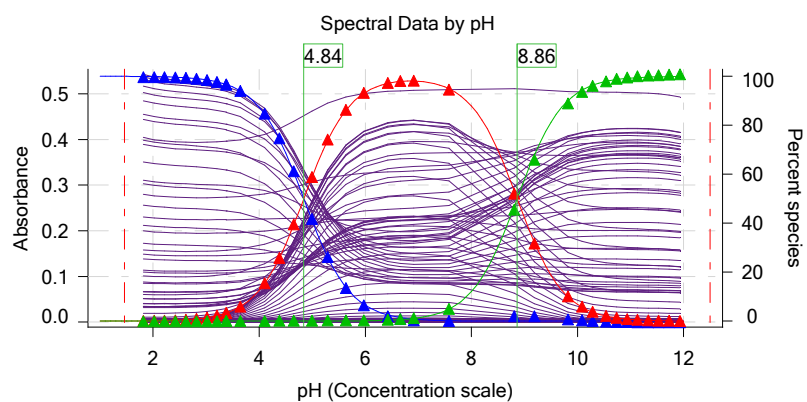
UV-metric pKa_0417936-0002   18E-22010   Assay 3 of 3

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	Pyridoxine HCl	5/22/2018 9:07:27 AM	User entered value
Sample by	Volume		Default value
Sample volume	0.0020 mL	5/22/2018 9:07:27 AM	User entered value
Solvent	DMSO		Default value
Sample concentration	0.048630 M	5/22/2018 9:07:27 AM	User entered value
Solubility	Unknown		Default value
Molecular weight	205.64	5/22/2018 9:07:35 AM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	2	5/22/2018 9:07:27 AM	User entered value
Sample is a	Ampholyte	5/22/2018 9:07:27 AM	User entered value
pKa 1	4.90	5/22/2018 9:07:27 AM	User entered value
Type	Base	5/22/2018 9:07:27 AM	User entered value

Multiset name: **0417936-0002**   Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
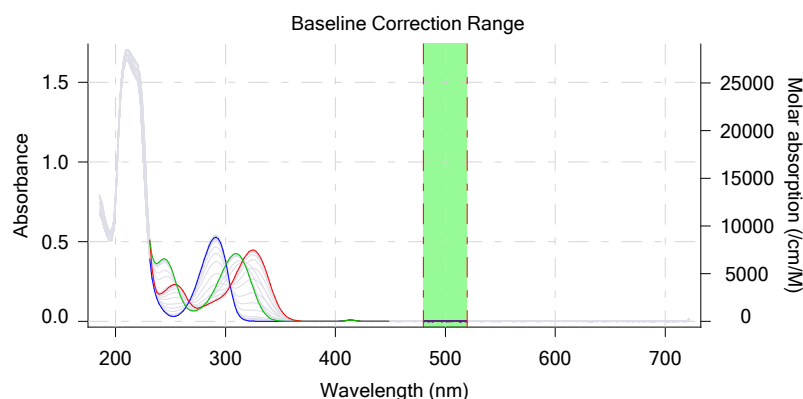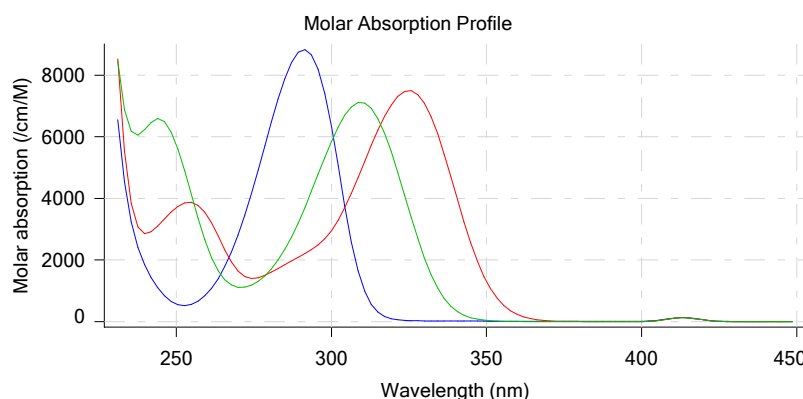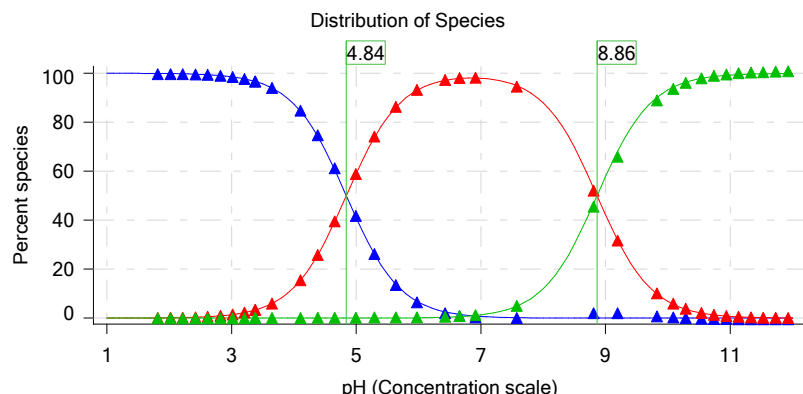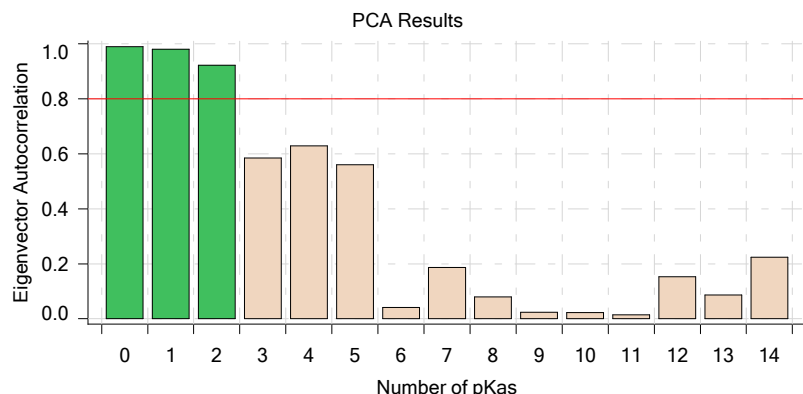Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_ISA_H2O_05_22_18.t3r**

Assay Model (continued)

Settings	Value	Date/Time changed	Imported from
pKa 2	8.80	5/22/2018 9:07:27 AM	User entered value
Type	Acid	5/22/2018 9:07:27 AM	User entered value
logp (XH2 +)	-10.00		Default value
logP (neutral XH)	-10.00	5/22/2018 9:07:27 AM	User entered value
logP (X -)	-10.00		Default value
Stoichiometry	1.00000		Default value
Aprotic counterion name	Chloride		From standards.xml file
Stoichiometry	1.00		From standards.xml file
Charge per counterion	-1		From standards.xml file

Events

Time	Event	Water	Acid	Base	Buffer	pH	dpH/dt	pH R-squared	pH SD
3:26.6	Dark spectrum								
3:28.1	Reference spectrum								
3:55.7	Volume reset due to vial change								
5:26.1	Initial pH = 7.04								
6:38.7	Data point 4	1.50000 mL	0.05007 mL	0.00000 mL	0.02500 mL	1.963	-0.00481	0.42832	0.000
7:07.5	Data point 5	1.50000 mL	0.05007 mL	0.01816 mL	0.02500 mL	2.161	-0.00197	0.09741	0.000
7:24.4	Data point 6	1.50000 mL	0.05007 mL	0.02949 mL	0.02500 mL	2.352	0.01775	0.77547	0.001
7:41.2	Data point 7	1.50000 mL	0.05007 mL	0.03671 mL	0.02500 mL	2.556	0.01447	0.91534	0.000
7:58.1	Data point 8	1.50000 mL	0.05007 mL	0.04116 mL	0.02500 mL	2.748	0.01707	0.90145	0.000
8:14.8	Data point 9	1.50000 mL	0.05007 mL	0.04403 mL	0.02500 mL	2.950	0.01943	0.95806	0.000
8:31.5	Data point 10	1.50000 mL	0.05007 mL	0.04581 mL	0.02500 mL	3.144	0.02281	0.96896	0.001
8:48.2	Data point 11	1.50000 mL	0.05007 mL	0.04694 mL	0.02500 mL	3.331	0.02811	0.92700	0.001
9:04.9	Data point 12	1.50000 mL	0.05007 mL	0.04767 mL	0.02500 mL	3.504	0.02972	0.96540	0.001
9:21.6	Data point 13	1.50000 mL	0.05007 mL	0.04817 mL	0.02500 mL	3.507	0.00665	0.76097	0.000
9:43.5	Data point 14	1.50000 mL	0.05007 mL	0.04878 mL	0.02500 mL	3.772	0.04680	0.93038	0.002
10:05.4	Data point 15	1.50000 mL	0.05007 mL	0.04932 mL	0.02500 mL	4.226	0.09266	0.89485	0.004
10:38.3	Data point 16	1.50000 mL	0.05007 mL	0.04962 mL	0.02500 mL	4.503	0.09339	0.87672	0.004
11:09.7	Data point 17	1.50000 mL	0.05007 mL	0.04976 mL	0.02500 mL	4.774	0.08508	0.87586	0.004
11:42.6	Data point 18	1.50000 mL	0.05007 mL	0.04988 mL	0.02500 mL	5.111	0.09044	0.88371	0.004
12:11.4	Data point 19	1.50000 mL	0.05007 mL	0.04998 mL	0.02500 mL	5.408	0.09053	0.87784	0.004
12:37.8	Data point 20	1.50000 mL	0.05007 mL	0.05007 mL	0.02500 mL	5.749	0.07504	0.76279	0.004
13:03.1	Data point 21	1.50000 mL	0.05007 mL	0.05016 mL	0.02500 mL	6.088	0.06956	0.63114	0.004
13:27.2	Data point 22	1.50000 mL	0.05007 mL	0.05031 mL	0.02500 mL	6.536	0.07530	0.63089	0.004
13:50.5	Data point 23	1.50000 mL	0.05007 mL	0.05042 mL	0.02500 mL	6.767	0.08426	0.77157	0.004
14:18.9	Data point 24	1.50000 mL	0.05007 mL	0.05054 mL	0.02500 mL	7.022	0.08110	0.79653	0.004
14:50.8	Data point 25	1.50000 mL	0.05007 mL	0.05073 mL	0.02500 mL	7.682	0.06344	0.65356	0.003
15:23.3	Data point 26	1.50000 mL	0.05007 mL	0.05094 mL	0.02500 mL	8.906	0.06293	0.52401	0.004
15:48.6	Data point 27	1.50000 mL	0.05007 mL	0.05111 mL	0.02500 mL	9.286	0.09036	0.80910	0.004
16:11.9	Data point 28	1.50000 mL	0.05007 mL	0.05139 mL	0.02500 mL	9.915	0.05262	0.79323	0.002
16:33.7	Data point 29	1.50000 mL	0.05007 mL	0.05172 mL	0.02500 mL	10.177	0.02012	0.73540	0.001
17:05.7	Data point 30	1.50000 mL	0.05007 mL	0.05212 mL	0.02500 mL	10.377	0.01988	0.79952	0.001
17:22.4	Data point 31	1.50000 mL	0.05007 mL	0.05278 mL	0.02500 mL	10.627	0.00863	0.54046	0.000
17:54.5	Data point 32	1.50000 mL	0.05007 mL	0.05402 mL	0.02500 mL	10.825	0.00628	0.56006	0.000
18:11.3	Data point 33	1.50000 mL	0.05007 mL	0.05581 mL	0.02500 mL	11.026	0.00555	0.65774	0.000
18:28.1	Data point 34	1.50000 mL	0.05007 mL	0.05863 mL	0.02500 mL	11.217	0.00337	0.31531	0.000
18:45.0	Data point 35	1.50000 mL	0.05007 mL	0.06305 mL	0.02500 mL	11.415	0.00239	0.31264	0.000
19:01.9	Data point 36	1.50000 mL	0.05007 mL	0.07013 mL	0.02500 mL	11.606	0.00493	0.59367	0.000
19:18.9	Data point 37	1.50000 mL	0.05007 mL	0.08130 mL	0.02500 mL	11.804	0.01334	0.90708	0.000
19:36.0	Data point 38	1.50000 mL	0.05007 mL	0.09948 mL	0.02500 mL	12.002	0.01147	0.83283	0.000
21:34.8	Assay volumes	1.75000 mL	0.15760 mL	0.09948 mL	0.02500 mL				

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				

Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_ISA_H2O_05_22_18.t3r**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Analyst name	Dorothy Levorse			
Separate reference vial	Yes			
Standard Experiment Settings				
Number of titrations	1			
Minimum pH	2.000			
Maximum pH	12.000			
pH step between points of	0.200			
Minimum titrant addition	0.00002 mL			
Maximum titrant addition	0.10000 mL			
Argon flow rate	100%			
Start titration using	Cautious pH adjust			
Advanced General Settings				
Detect turbidity using	Spectrometer			
Monitor at a wavelength of	500.0 nm			
Absorbance threshold of	0.100			
Collect turbidity sensor data	No			
Stir after titrant addition for	5 seconds			
For titrant addition, stir at	15%			
Titrant Pre-Dose				
Titrant pre-dose	None			
Assay Medium				
Cosolvent in use	No			
ISA water volume	1.50 mL			
Water added	Automatic			
After water addition, stir for	5 seconds			
At a speed of	15%			
Buffer in use	Yes			
Buffer type	Phosphate Buffer			
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			
After medium addition, stir for	5 seconds			
Sample Sonication				
Sonicate	No			
Sample Dissolution				
Perform a dissolution stage	No			
Carbonate purge				
Perform a carbonate purge	No			
Temperature Control				
Wait for temperature	Yes			
Required start temperature	25.0°C			
Acceptable deviation	0.5°C			
Time to wait	60 seconds			
Stir speed of	15%			
Titration 1				
Titrate from	Low to high pH			
Adjust to start pH	Yes			
After pH adjust stir for	10 seconds			
Data Point Stability				
Stir during data point collection	Yes			
For point collection, stir at	15%			
Delay before data point collection	0 seconds			
Number of points to average	20 points			
Time interval between points	0.50 seconds			
Required maximum standard deviation	0.00500 dpH/dt			
Stability timeout after	60 seconds			
Experiment cleanup				
Adjust pH to cleanup	To start pH			
And then stir for	60 seconds			
For cleaning, stir at	20%			

Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_ISA_H2O_05_22_18.t3r**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Then add water volume	0.25 mL			
And then stir for	30 seconds			

Calibration Settings

Setting	Value	Date/Time changed	Imported from
Four-Plus alpha	0.144	5/22/2018 11:56:48 AM	C:\Sirius_T3\18E-22009_Blank standardisation.t3r
Four-Plus S	0.9948	5/22/2018 11:56:48 AM	C:\Sirius_T3\18E-22009_Blank standardisation.t3r
Four-Plus jH	1.0	5/22/2018 11:56:48 AM	C:\Sirius_T3\18E-22009_Blank standardisation.t3r
Four-Plus jOH	-0.8	5/22/2018 11:56:48 AM	C:\Sirius_T3\18E-22009_Blank standardisation.t3r
Base concentration factor	1.012	5/22/2018 11:56:49 AM	C:\Sirius_T3\KOH18D10.t3r
Acid concentration factor	0.998	5/22/2018 11:56:49 AM	C:\Sirius_T3\18E-22009_Blank standardisation.t3r

Instrument Settings

Setting	Value	Batch Id	Install date
Instrument owner	Merck		
Instrument ID	T311053		
Instrument type	T3 Simulator		
Software version	1.1.3.0		
Dispenser module		T3DM1100253	3/31/2009 6:24:52 AM
Dispenser 0	Water		3/31/2009 6:25:05 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Water (0.15 M KCl)	2-6-18	5/15/2018 2:12:22 PM
Dispenser 2	Acid		3/31/2009 6:25:11 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Acid (0.5 M HCl)	3-22-18	5/15/2018 2:12:48 PM
Dispenser 1	Base		3/31/2009 6:25:21 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Base (0.5 M KOH)	3-22-18	5/15/2018 2:12:34 PM
Dispenser 5	Cosolvent		3/31/2009 6:26:24 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Distribution valve 5	Distribution Valve		3/31/2009 6:28:19 AM
Firmware version	1.1.3		
Port A	Methanol (80%, 0.15 M KCl)	2-8-18	5/15/2018 2:14:14 PM
Port B	Cyclohexane		4/10/2018 8:40:51 AM
Port C	MeCN (50%, 0.15 M KCl)	4-16-18	5/15/2018 2:14:20 PM
Dispenser 3	Buffer		8/3/2010 6:05:16 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Dodecane	1-31-2018	5/15/2018 2:12:54 PM
Dispenser 6	Octanol		10/22/2010 11:52:43 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Octanol	1-31-2018	4/9/2018 9:14:11 AM
Titrator		T3TM1100153	3/31/2009 6:24:17 AM
Horizontal axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Probe I/O firmware version	1.1.1		
Electrode	T3 Electrode	T3E0769	8/15/2017 10:21:54 AM
E0 calibration	-9.70 mV		5/22/2018 11:57:16 AM
Filling solution	3M KCl	KCL095	5/21/2018 8:57:01 AM
Liquids			
Wash 1	50% IPA:50% Water		5/22/2018 8:38:15 AM
Wash 2	0.5% Trition X-100 in H20		5/22/2018 8:38:18 AM

Multiset name: **0417936-0002**   Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_ISA_H2O_05_22_18.t3r**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Buffer position 1	pH7 Wash		5/22/2018 8:38:22 AM
Buffer position 2	pH 7		5/22/2018 8:38:25 AM
Storage position			5/22/2018 8:38:32 AM
Wash water	3.6e+003 mL	5-15-18	5/15/2018 2:11:48 PM
Waste	6.9e+003 mL		3/19/2018 10:48:12 AM
Temperature controller			8/5/2010 7:35:13 AM
Turbidity detector			3/31/2009 6:24:45 AM
Spectrometer		072390	11/23/2010 12:22:28 PM
Dip probe		11086	
Wavelength coefficient A0	185.563		
Wavelength coefficient A1	2.17439		
Wavelength coefficient A2	-0.000285622		
Total lamp lit time	897:26:49		11/23/2010 12:22:28 PM
Calibrated on	5/21/2018 2:44:22 PM		
Integration time	19		
Scans averaged	10		
Autoloader		T3AL1100237	11/10/2015 10:34:13 AM
Left-right axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Front-back axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Configuration			
Alternate titration position	Titration position		
Alternate reference position	Reference position		
Maximum standard vial volume	3.50 mL		
Maximum alternate vial volume	25.00 mL		
Automatic action idle period	5 minute(s)		
Titrant tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		
Flowing wash stir speed	30%		
Solvent wash stir duration	5 s		
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		
E0 calibration reading stir speed	0%		
Spectrometer calibration stir duration	5 s		
Spectrometer calibration stir speed	30%		
Spectrometer calibration wash pump volume	20.0 mL		
Spectrometer calibration wash stir duration	5 s		
Spectrometer calibration wash stir speed	30%		
Overhead dispense height	10000		

Refinement Settings

Setting	Value	Default value
Turbidity detection method	Spectrometer	Spectrometer
Turbidity wavelength to assess	500.0 nm	500.0 nm
Turbidity maximum absorbance	0.100	0.100
Turbidity probe threshold	50.00	50.00
Exclude turbid points	Yes	Yes

Multiset name: **0417936-0002**   Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_ISA_H2O_05_22_18.t3r**

Refinement Settings (continued)

Setting	Value	Default value
Low intensity warning threshold	100	100
Minimum absorbance change threshold	0.100	0.100
Eigenvector autocorrelation threshold	0.80	0.80
Maximum RMSD severe warning	0.250	0.250
Maximum RMSD warning	0.050	0.050

Experiment Log

[1:27] Air gap released for Acid (0.5 M HCl)
[2:07] Air gap created for Water (0.15 M KCl)
[2:08] Air gap created for Acid (0.5 M HCl)
[2:08] Air gap created for Base (0.5 M KOH)
[2:08] Air gap released for Water (0.15 M KCl)
[2:13] Titrator arm moved to Reference position
[2:13] Argon flow rate set to 100
[2:13] Preparing reference vial
[2:13] Automatically add 1.50000 mL of water
[2:38] Dispensed 1.500000 mL of Water (0.15 M KCl)
[2:38] Stirrer speed set to 15
[2:48] Iterative adjust 7.74 -> 2.00
[2:48] pH 7.74 -> 2.00
[2:50] Air gap released for Acid (0.5 M HCl)
[2:51] Dispensed 0.043462 mL of Acid (0.5 M HCl)
[2:56] pH 2.07 -> 2.00
[2:56] Dispensed 0.006609 mL of Acid (0.5 M HCl)
[3:01] Stirrer speed set to 0
[3:05] Titrator arm moved over Reference position
[3:05] Air gap created for Water (0.15 M KCl)
[3:06] Air gap created for Acid (0.5 M HCl)
[3:09] Titrator arm moved to Reference position
[3:10] Air gap released for Water (0.15 M KCl)
[3:10] Stirrer speed set to 15
[3:25] Stirrer speed set to 0
[3:26] Dark scan collected
[3:28] Reference scan collected
[3:55] Probes washed
[3:55] Volume reset due to vial change
[4:04] Titrator arm moved to Titration position
[4:04] Preparing sample vial
[4:04] Automatically add 1.50000 mL of water
[5:16] Dispensed 1.500000 mL of Water (0.15 M KCl)
[5:16] Stirrer speed set to 15
[5:26] Initial pH = 7.04
[5:26] Adding reagent volumes used in reference
[5:26]   Adding acid volume of 0.0500706
[5:27] Air gap released for Acid (0.5 M HCl)
[5:28] Dispensed 0.050071 mL of Acid (0.5 M HCl)
[6:50] Datapoint id 4 collected
[6:50] pH 1.96 -> 2.16
[6:50] Using cautious pH adjust
[6:51] Air gap released for Base (0.5 M KOH)
[6:51] Dispensed 0.009102 mL of Base (0.5 M KOH)
[6:56] Stepping pH = 2.05
[6:57] Dispensed 0.007079 mL of Base (0.5 M KOH)
[7:02] Stepping pH = 2.13
[7:02] Dispensed 0.001976 mL of Base (0.5 M KOH)
[7:07] Stepping pH = 2.16
[7:19] Datapoint id 5 collected
[7:19] Charge balance equation is out by 0.3%

Multiset name: **0417936-0002** Instrument ID: **T311053**

Analyst: **Dorothy Levorse**

Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_ISA_H2O_05_22_18.t3r**

Experiment Log (continued)

[7:19] pH 2.16 -> 2.36
[7:19] Using charge balance adjust
[7:19] Dispensed 0.011336 mL of Base (0.5 M KOH)
[7:35] Datapoint id 6 collected
[7:35] Charge balance equation is out by -4.8%
[7:35] pH 2.35 -> 2.55
[7:35] Using charge balance adjust
[7:36] Dispensed 0.007220 mL of Base (0.5 M KOH)
[7:52] Datapoint id 7 collected
[7:52] Charge balance equation is out by 2.4%
[7:52] pH 2.56 -> 2.76
[7:52] Using charge balance adjust
[7:53] Dispensed 0.004445 mL of Base (0.5 M KOH)
[8:09] Datapoint id 8 collected
[8:09] Charge balance equation is out by -4.0%
[8:09] pH 2.75 -> 2.95
[8:09] Using charge balance adjust
[8:09] Dispensed 0.002869 mL of Base (0.5 M KOH)
[8:26] Datapoint id 9 collected
[8:26] Charge balance equation is out by 1.0%
[8:26] pH 2.95 -> 3.15
[8:26] Using charge balance adjust
[8:26] Dispensed 0.001787 mL of Base (0.5 M KOH)
[8:43] Datapoint id 10 collected
[8:43] Charge balance equation is out by -3.4%
[8:43] pH 3.14 -> 3.34
[8:43] Using charge balance adjust
[8:43] Dispensed 0.001129 mL of Base (0.5 M KOH)
[8:59] Datapoint id 11 collected
[8:59] Charge balance equation is out by -6.2%
[8:59] pH 3.33 -> 3.53
[8:59] Using charge balance adjust
[8:59] Dispensed 0.000729 mL of Base (0.5 M KOH)
[9:16] Datapoint id 12 collected
[9:16] Charge balance equation is out by -13.8%
[9:16] pH 3.50 -> 3.70
[9:16] Using charge balance adjust
[9:16] Dispensed 0.000494 mL of Base (0.5 M KOH)
[9:33] Datapoint id 13 collected
[9:33] Charge balance equation is out by -98.1%
[9:33] pH 3.51 -> 3.71
[9:33] Using cautious pH adjust
[9:33] Dispensed 0.000259 mL of Base (0.5 M KOH)
[9:38] Stepping pH = 3.56
[9:38] Dispensed 0.000353 mL of Base (0.5 M KOH)
[9:43] Stepping pH = 3.77
[9:55] Datapoint id 14 collected
[9:55] Charge balance equation is out by 22.1%
[9:55] pH 3.77 -> 3.97
[9:55] Using cautious pH adjust
[9:55] Dispensed 0.000141 mL of Base (0.5 M KOH)
[10:00] Stepping pH = 3.78
[10:00] Dispensed 0.000400 mL of Base (0.5 M KOH)
[10:05] Stepping pH = 4.21
[10:17] Datapoint id 15 collected
[10:17] Charge balance equation is out by 95.5%
[10:17] pH 4.23 -> 4.43
[10:17] Using cautious pH adjust
[10:17] Dispensed 0.000047 mL of Base (0.5 M KOH)
[10:22] Stepping pH = 4.23

Multiset name: **0417936-0002**   Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_ISA_H2O_05_22_18.t3r**

Experiment Log (continued)

[10:23] Dispensed 0.000165 mL of Base (0.5 M KOH)
[10:28] Stepping pH = 4.35
[10:28] Dispensed 0.000071 mL of Base (0.5 M KOH)
[10:33] Stepping pH = 4.41
[10:33] Dispensed 0.000024 mL of Base (0.5 M KOH)
[10:38] Stepping pH = 4.46
[10:54] Datapoint id 16 collected
[10:54] Charge balance equation is out by 177.6%
[10:54] pH 4.50 -> 4.70
[10:54] Using cautious pH adjust
[10:54] Dispensed 0.000024 mL of Base (0.5 M KOH)
[10:59] Stepping pH = 4.51
[10:59] Dispensed 0.000094 mL of Base (0.5 M KOH)
[11:04] Stepping pH = 4.66
[11:04] Dispensed 0.000024 mL of Base (0.5 M KOH)
[11:09] Stepping pH = 4.72
[11:27] Datapoint id 17 collected
[11:27] Charge balance equation is out by 122.5%
[11:27] pH 4.77 -> 4.97
[11:27] Using cautious pH adjust
[11:27] Dispensed 0.000024 mL of Base (0.5 M KOH)
[11:32] Stepping pH = 4.78
[11:32] Dispensed 0.000071 mL of Base (0.5 M KOH)
[11:37] Stepping pH = 4.95
[11:37] Dispensed 0.000024 mL of Base (0.5 M KOH)
[11:42] Stepping pH = 5.03
[12:01] Datapoint id 18 collected
[12:01] Charge balance equation is out by 129.0%
[12:01] pH 5.11 -> 5.31
[12:01] Using cautious pH adjust
[12:01] Dispensed 0.000024 mL of Base (0.5 M KOH)
[12:06] Stepping pH = 5.12
[12:06] Dispensed 0.000071 mL of Base (0.5 M KOH)
[12:11] Stepping pH = 5.35
[12:27] Datapoint id 19 collected
[12:27] Charge balance equation is out by 92.0%
[12:27] pH 5.41 -> 5.61
[12:27] Using cautious pH adjust
[12:27] Dispensed 0.000024 mL of Base (0.5 M KOH)
[12:32] Stepping pH = 5.42
[12:32] Dispensed 0.000071 mL of Base (0.5 M KOH)
[12:37] Stepping pH = 5.70
[12:52] Datapoint id 20 collected
[12:52] Charge balance equation is out by 92.4%
[12:52] pH 5.75 -> 5.95
[12:52] Using cautious pH adjust
[12:52] Dispensed 0.000024 mL of Base (0.5 M KOH)
[12:57] Stepping pH = 5.75
[12:58] Dispensed 0.000071 mL of Base (0.5 M KOH)
[13:03] Stepping pH = 6.05
[13:17] Datapoint id 21 collected
[13:17] Charge balance equation is out by 95.0%
[13:17] pH 6.09 -> 6.29
[13:17] Using cautious pH adjust
[13:17] Dispensed 0.000024 mL of Base (0.5 M KOH)
[13:22] Stepping pH = 6.09
[13:22] Dispensed 0.000118 mL of Base (0.5 M KOH)
[13:27] Stepping pH = 6.51
[13:40] Datapoint id 22 collected
[13:40] Charge balance equation is out by 199.0%

Multiset name: **0417936-0002**   Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_ISA_H2O_05_22_18.t3r**

Experiment Log (continued)

[13:40] pH 6.54 -> 6.74
[13:40] Using cautious pH adjust
[13:40] Dispensed 0.000024 mL of Base (0.5 M KOH)
[13:45] Stepping pH = 6.53
[13:45] Dispensed 0.000094 mL of Base (0.5 M KOH)
[13:50] Stepping pH = 6.74
[14:03] Datapoint id 23 collected
[14:03] Charge balance equation is out by 215.5%
[14:03] pH 6.77 -> 6.97
[14:03] Using cautious pH adjust
[14:03] Dispensed 0.000024 mL of Base (0.5 M KOH)
[14:08] Stepping pH = 6.77
[14:08] Dispensed 0.000071 mL of Base (0.5 M KOH)
[14:13] Stepping pH = 6.93
[14:13] Dispensed 0.000024 mL of Base (0.5 M KOH)
[14:18] Stepping pH = 6.97
[14:35] Datapoint id 24 collected
[14:35] Charge balance equation is out by 308.2%
[14:35] pH 7.02 -> 7.22
[14:35] Using cautious pH adjust
[14:35] Dispensed 0.000024 mL of Base (0.5 M KOH)
[14:40] Stepping pH = 7.02
[14:40] Dispensed 0.000047 mL of Base (0.5 M KOH)
[14:45] Stepping pH = 7.03
[14:45] Dispensed 0.000118 mL of Base (0.5 M KOH)
[14:50] Stepping pH = 7.57
[15:07] Datapoint id 25 collected
[15:07] Charge balance equation is out by 983.6%
[15:07] pH 7.68 -> 7.88
[15:07] Using cautious pH adjust
[15:07] Dispensed 0.000024 mL of Base (0.5 M KOH)
[15:13] Stepping pH = 7.68
[15:13] Dispensed 0.000024 mL of Base (0.5 M KOH)
[15:18] Stepping pH = 7.67
[15:18] Dispensed 0.000165 mL of Base (0.5 M KOH)
[15:23] Stepping pH = 8.80
[15:38] Datapoint id 26 collected
[15:38] Charge balance equation is out by 1,615.7%
[15:38] pH 8.91 -> 9.11
[15:38] Using cautious pH adjust
[15:38] Dispensed 0.000024 mL of Base (0.5 M KOH)
[15:43] Stepping pH = 8.90
[15:43] Dispensed 0.000141 mL of Base (0.5 M KOH)
[15:48] Stepping pH = 9.26
[16:01] Datapoint id 27 collected
[16:01] Charge balance equation is out by 202.8%
[16:01] pH 9.29 -> 9.49
[16:01] Using cautious pH adjust
[16:01] Dispensed 0.000047 mL of Base (0.5 M KOH)
[16:06] Stepping pH = 9.29
[16:06] Dispensed 0.000235 mL of Base (0.5 M KOH)
[16:11] Stepping pH = 9.91
[16:23] Datapoint id 28 collected
[16:23] Charge balance equation is out by 196.1%
[16:23] pH 9.92 -> 10.12
[16:23] Using cautious pH adjust
[16:23] Dispensed 0.000118 mL of Base (0.5 M KOH)
[16:28] Stepping pH = 9.96
[16:28] Dispensed 0.000212 mL of Base (0.5 M KOH)
[16:33] Stepping pH = 10.17

Multiset name: **0417936-0002**   Instrument ID: **T311053**
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Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_ISA_H2O_05_22_18.t3r**

Experiment Log (continued)

[16:45] Datapoint id 29 collected
[16:45] Charge balance equation is out by 34.5%
[16:45] pH 10.18 -> 10.38
[16:45] Using cautious pH adjust
[16:45] Dispensed 0.000212 mL of Base (0.5 M KOH)
[16:50] Stepping pH = 10.31
[16:50] Dispensed 0.000094 mL of Base (0.5 M KOH)
[16:55] Stepping pH = 10.34
[16:55] Dispensed 0.000071 mL of Base (0.5 M KOH)
[17:00] Stepping pH = 10.37
[17:00] Dispensed 0.000024 mL of Base (0.5 M KOH)
[17:05] Stepping pH = 10.37
[17:17] Datapoint id 30 collected
[17:17] Charge balance equation is out by 3.1%
[17:17] pH 10.38 -> 10.58
[17:17] Using charge balance adjust
[17:17] Dispensed 0.000659 mL of Base (0.5 M KOH)
[17:33] Datapoint id 31 collected
[17:33] Charge balance equation is out by 25.0%
[17:33] pH 10.63 -> 10.83
[17:33] Using cautious pH adjust
[17:34] Dispensed 0.000564 mL of Base (0.5 M KOH)
[17:39] Stepping pH = 10.73
[17:39] Dispensed 0.000423 mL of Base (0.5 M KOH)
[17:44] Stepping pH = 10.80
[17:44] Dispensed 0.000165 mL of Base (0.5 M KOH)
[17:49] Stepping pH = 10.82
[17:49] Dispensed 0.000094 mL of Base (0.5 M KOH)
[17:54] Stepping pH = 10.82
[18:06] Datapoint id 32 collected
[18:06] Charge balance equation is out by 9.2%
[18:06] pH 10.82 -> 11.02
[18:06] Using charge balance adjust
[18:06] Dispensed 0.001787 mL of Base (0.5 M KOH)
[18:22] Datapoint id 33 collected
[18:22] Charge balance equation is out by 0.4%
[18:22] pH 11.03 -> 11.23
[18:22] Using charge balance adjust
[18:23] Dispensed 0.002822 mL of Base (0.5 M KOH)
[18:39] Datapoint id 34 collected
[18:39] Charge balance equation is out by -4.5%
[18:39] pH 11.22 -> 11.42
[18:39] Using charge balance adjust
[18:39] Dispensed 0.004421 mL of Base (0.5 M KOH)
[18:56] Datapoint id 35 collected
[18:56] Charge balance equation is out by -0.8%
[18:56] pH 11.42 -> 11.62
[18:56] Using charge balance adjust
[18:56] Dispensed 0.007079 mL of Base (0.5 M KOH)
[19:13] Datapoint id 36 collected
[19:13] Charge balance equation is out by -4.4%
[19:13] pH 11.61 -> 11.81
[19:13] Using charge balance adjust
[19:13] Dispensed 0.011171 mL of Base (0.5 M KOH)
[19:30] Datapoint id 37 collected
[19:30] Charge balance equation is out by -0.9%
[19:30] pH 11.80 -> 12.00
[19:30] Using charge balance adjust
[19:30] Dispensed 0.018180 mL of Base (0.5 M KOH)
[19:47] Datapoint id 38 collected

Multiset name: **0417936-0002**   Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_ISA_H2O_05_22_18.t3r**

Experiment Log (continued)

[19:47] Charge balance equation is out by -1.3%
[19:47] Cleaning up
[19:47] Iterative adjust 12.00 -> 2.00
[19:47] pH 12.00 -> 2.00
[19:47] Stirrer speed set to 20
[19:49] Dispensed 0.097342 mL of Acid (0.5 M HCl)
[19:54] pH 2.10 -> 2.00
[19:55] Dispensed 0.010183 mL of Acid (0.5 M HCl)
[20:00] Holding pH 2.00
[21:04] Dispensed 0.250000 mL of Water (0.15 M KCl)
[21:04] Iterative adjust 2.00 -> 2.00
[21:04] Holding pH 2.00
[21:34] Stirrer speed set to 0
[21:34] Argon flow rate set to 0

Tray Information

Title
Location   A5